Propanoic acid, phenylmethyl ester

Other names:	Benzyl n-propionate
	Benzyl propionate
	benzyl propanoate
	propionic acid, benzyl ester
Inchi:	InChI=1S/C10H12O2/c1-2-10(11)12-8-9-6-4-3-5-7-9/h3-7H,2,8H2,1H3
InchiKey:	VHOMAPWVLKRQAZ-UHFFFAOYSA-N
Formula:	C10H12O2
SMILES:	CCC(=O)OCc1ccccc1
Mol. weight [g/mol]:	164.20
CAS:	122-63-4

Physical Properties

Property code	Value	Unit	Source
gf	-88.19	kJ/mol	Joback Method
hf	-258.00	kJ/mol	Joback Method
hfus	18.48	kJ/mol	Joback Method
hvap	49.29	kJ/mol	Joback Method
log10ws	-2.47		Crippen Method
logp	2.140		Crippen Method
mcvol	135.440	ml/mol	McGowan Method
pc	3082.99	kPa	Joback Method
rinpol	1284.00		NIST Webbook
rinpol	1225.00		NIST Webbook
rinpol	1250.00		NIST Webbook
rinpol	1237.00		NIST Webbook
rinpol	1227.90		NIST Webbook
rinpol	1224.40		NIST Webbook
rinpol	1225.00		NIST Webbook
rinpol	1234.00		NIST Webbook
rinpol	1224.40		NIST Webbook
rinpol	1266.20		NIST Webbook
rinpol	1230.40		NIST Webbook
rinpol	1255.00		NIST Webbook
rinpol	1284.00		NIST Webbook
rinpol	1266.00		NIST Webbook
rinpol	1257.00		NIST Webbook
rinpol	1250.00		NIST Webbook

rinpol	1230.40		NIST Webbook
rinpol	1245.00		NIST Webbook
rinpol	1245.00		NIST Webbook
rinpol	1259.00		NIST Webbook
rinpol	1272.00		NIST Webbook
rinpol	1225.00		NIST Webbook
ripol	1784.40		NIST Webbook
ripol	1766.00		NIST Webbook
ripol	1769.00		NIST Webbook
ripol	1787.90		NIST Webbook
ripol	1775.00		NIST Webbook
ripol	1791.00		NIST Webbook
ripol	1784.40		NIST Webbook
ripol	1775.00		NIST Webbook
ripol	1791.00		NIST Webbook
ripol	1783.00		NIST Webbook
ripol	1787.90		NIST Webbook
ripol	1784.70		NIST Webbook
tb	531.17	K	Joback Method
tc	743.85	K	Joback Method
tf	301.04	K	Joback Method
vc	0.511	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	350.35	J/mol×K	672.95	Joback Method
cpg	361.01	J/mol×K	708.40	Joback Method
cpg	300.47	J/mol×K	531.17	Joback Method
cpg	314.07	J/mol×K	566.62	Joback Method
cpg	326.90	J/mol×K	602.06	Joback Method
cpg	338.99	J/mol×K	637.51	Joback Method
cpg	370.98	J/mol×K	743.85	Joback Method

dvisc	0.0015150	Pa×s	318.15	Densities and Viscosities of Binary Mixtures of Ethyl Acetoacetate, Ethyl Isovalerate, Methyl Benzoate, Benzyl Acetate, Ethyl Salicylate, and Benzyl Propionate with Ethanol at T) (288.15, 298.15, 308.15, and 318.15) K
dvisc	0.0017870	Pa×s	308.15	Densities and Viscosities of Binary Mixtures of Ethyl Acetoacetate, Ethyl Isovalerate, Methyl Benzoate, Benzyl Acetate, Ethyl Salicylate, and Benzyl Propionate with Ethanol at T) (288.15, 298.15, 308.15, and 318.15) K
dvisc	0.0021230	Pa×s	298.15	Densities and Viscosities of Binary Mixtures of Ethyl Acetoacetate, Ethyl Isovalerate, Methyl Benzoate, Benzyl Acetate, Ethyl Salicylate, and Benzyl Propionate with Ethanol at T) (288.15, 298.15, 308.15, and 318.15) K
dvisc	0.0025500	Pa×s	288.15	Densities and Viscosities of Binary Mixtures of Ethyl Acetoacetate, Ethyl Isovalerate, Methyl Benzoate, Benzyl Acetate, Ethyl Salicylate, and Benzyl Propionate with Ethanol at T) (288.15, 298.15, 308.15, and 318.15) K
hvapt	59.00	kJ/mol	338.00	NIST Webbook

rhol	1027.60	kg/m3	298.15	Refractive Indices and Surface Tensions of Binary Mixtures of Ethyl Acetoacetate, Ethyl Isovalerate, Methyl Benzoate, Benzyl Acetate, Ethyl Salicylate, and Benzyl Propionate with Ethanol at (288.15, 298.15, 308.15, and 318.15) K
srf	0.03	N/m	358.15	Densities, Viscosities, Refractive Indices, and Surface Tensions for 12 Flavor Esters from T) 288.15 K to T) 358.15 K
srf	0.03	N/m	348.15	Densities, Viscosities, Refractive Indices, and Surface Tensions for 12 Flavor Esters from T) 288.15 K to T) 358.15 K
srf	0.03	N/m	338.15	Densities, Viscosities, Refractive Indices, and Surface Tensions for 12 Flavor Esters from T) 288.15 K to T) 358.15 K
srf	0.03	N/m	328.15	Densities, Viscosities, Refractive Indices, and Surface Tensions for 12 Flavor Esters from T) 288.15 K to T) 358.15 K
srf	0.03	N/m	318.15	Densities, Viscosities, Refractive Indices, and Surface Tensions for 12 Flavor Esters from T) 288.15 K to T) 358.15 K

srf	0.03	N/m	308.15	Densities, Viscosities, Refractive Indices, and Surface Tensions for 12 Flavor Esters from T) 288.15 K to T) 358.15 K
srf	0.03	N/m	298.15	Densities, Viscosities, Refractive Indices, and Surface Tensions for 12 Flavor Esters from T) 288.15 K to T) 358.15 K
srf	0.04	N/m	288.15	Densities, Viscosities, Refractive Indices, and Surface Tensions for 12 Flavor Esters from T) 288.15 K to T) 358.15 K

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Densities, Viscosities, Refractive Indices, and Surface Tensions for 12 Flavor Esters from T) 288.15 K to T) 358.15 K:	https://www.doi.org/10.1021/je050170x
Densities and Viscosities of Binary Mixtures of Ethyl Acetoacetate, Ethyl Isovalerate, Methyl Benzoate, Benzyl Acetate, Ethyl Salicylate, and Benzyl Propionate with Ethanol at T) (288.15, 298.15, and 318.15) K:	https://www.doi.org/10.1021/je050402s
Refractive Indices and Surface Tensions of Binary Mixtures of Ethyl Acetoacetate, Ethyl Isovalerate, Methyl Benzoate, Benzyl Acetate, Ethyl Salicylate, and Benzyl Propionate with Ethanol at (288.15, 298.15, 308.15, and 318.15) K:	https://www.doi.org/10.1021/je060139a
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Rotzowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C122634&Units=SI

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions

hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rhol:	Liquid Density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
srf:	Surface Tension
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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