

Propanoic acid, 2-phenylethyl ester

Other names:	2-Phenethyl propionate
	2-Phenyl ethyl propanoate
	2-Phenylethanol, propanoate
	2-phenylethyl propanoate
	2-phenylethyl propionate
	Benzylcarbiny propionate
	ENT 18544
	EcoPCO ACU
	NSC 404457
	Phenethyl alcohol, propionate
	Phenethyl propanoate
	Phenethyl propionate
	Phenylethyl n-propionate
	Phenylethyl propanoate
	Phenylethyl propionate
	Propionic acid, 2-phenylethyl ester
	Propionic acid, phenethyl ester
	«beta»-Phenylethyl propionate
Inchi:	InChI=1S/C11H14O2/c1-2-11(12)13-9-8-10-6-4-3-5-7-10/h3-7H,2,8-9H2,1H3
InchiKey:	HVGZQCSMLUDISR-UHFFFAOYSA-N
Formula:	C11H14O2
SMILES:	CCC(=O)OCCc1ccccc1
Mol. weight [g/mol]:	178.23
CAS:	122-70-3

Physical Properties

Property code	Value	Unit	Source
gf	-79.77	kJ/mol	Joback Method
hf	-278.64	kJ/mol	Joback Method
hfus	21.07	kJ/mol	Joback Method
hvap	51.51	kJ/mol	Joback Method
log10ws	-2.39		Crippen Method
logp	2.182		Crippen Method
mcvol	149.530	ml/mol	McGowan Method
pc	2778.85	kPa	Joback Method
rinpol	1349.00		NIST Webbook
rinpol	1356.00		NIST Webbook

rinpol	1315.00		NIST Webbook
rinpol	1350.00		NIST Webbook
rinpol	1350.00		NIST Webbook
rinpol	1350.00		NIST Webbook
rinpol	1350.00		NIST Webbook
rinpol	1353.00		NIST Webbook
rinpol	1353.70		NIST Webbook
rinpol	1353.00		NIST Webbook
rinpol	1350.00		NIST Webbook
rinpol	1325.00		NIST Webbook
rinpol	1353.70		NIST Webbook
rinpol	1350.00		NIST Webbook
rinpol	1309.00		NIST Webbook
rinpol	1328.00		NIST Webbook
rinpol	1325.00		NIST Webbook
rinpol	1353.00		NIST Webbook
tb	554.05	K	Joback Method
tc	763.32	K	Joback Method
tf	312.31	K	Joback Method
vc	0.568	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	421.37	J/mol×K	763.32	Joback Method
cpg	410.76	J/mol×K	728.44	Joback Method
cpg	399.42	J/mol×K	693.56	Joback Method
cpg	387.33	J/mol×K	658.68	Joback Method
cpg	374.48	J/mol×K	623.81	Joback Method
cpg	360.84	J/mol×K	588.93	Joback Method
cpg	346.39	J/mol×K	554.05	Joback Method
dvisc	0.0023060	Pa×s	312.31	Joback Method
dvisc	0.0002006	Pa×s	554.05	Joback Method
dvisc	0.0002569	Pa×s	513.76	Joback Method
dvisc	0.0003432	Pa×s	473.47	Joback Method
dvisc	0.0004838	Pa×s	433.18	Joback Method
dvisc	0.0007317	Pa×s	392.89	Joback Method
dvisc	0.0012165	Pa×s	352.60	Joback Method

hvapt	65.60	kJ/mol	298.15	Vapor pressures and vaporization enthalpies of a series of esters used in flavors by correlation gas chromatography
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Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C122703&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Vapor pressures and vaporization enthalpies of a series of esters used in flavors by correlation gas chromatography:	https://www.doi.org/10.1016/j.jct.2015.02.015
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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