«beta»-Phenylethyl butyrate

Other names:	2-Phenethyl butanoate
	2-phenylethyl butanoate
	2-phenylethyl butyrate
	Benzylcarbinyl butyrate
	Butanoic acid, 2-phenylethyl ester
	Butyric acid, phenethyl ester
	Phenethyl butanoate
	Phenylethyl butyrate
	phenethyl butyrate
	«beta»-Phenethyl n-butanoate
	«beta»-Phenylethyl n-butyrate
Inchi:	InChI=1S/C12H16O2/c1-2-6-12(13)14-10-9-11-7-4-3-5-8-11/h3-5,7-8H,2,6,9-10H2,1H3
InchiKey:	WFNDDSQUKATKNX-UHFFFAOYSA-N
Formula:	C12H16O2
SMILES:	CCCC(=O)OCCc1ccccc1
Mol. weight [g/mol]:	192.25
CAS:	103-52-6

Physical Properties

Property code	Value	Unit	Source
gf	-71.35	kJ/mol	Joback Method
hf	-299.28	kJ/mol	Joback Method
hfus	23.66	kJ/mol	Joback Method
hvap	53.74	kJ/mol	Joback Method
log10ws	-2.81		Crippen Method
logp	2.572		Crippen Method
mcvol	163.620	ml/mol	McGowan Method
pc	2517.59	kPa	Joback Method
rinpol	1422.00		NIST Webbook
rinpol	1440.00		NIST Webbook
rinpol	1405.00		NIST Webbook
rinpol	1440.00		NIST Webbook
rinpol	1446.00		NIST Webbook
rinpol	1444.40		NIST Webbook
rinpol	1431.00		NIST Webbook
rinpol	1447.00		NIST Webbook
rinpol	1447.00		NIST Webbook

rinpol	1439.00		NIST Webbook
rinpol	1411.00		NIST Webbook
rinpol	1429.00		NIST Webbook
rinpol	1439.00		NIST Webbook
rinpol	1449.00		NIST Webbook
rinpol	1457.00		NIST Webbook
rinpol	1447.00		NIST Webbook
rinpol	1422.00		NIST Webbook
rinpol	1415.00		NIST Webbook
ripol	1958.00		NIST Webbook
ripol	1930.00		NIST Webbook
ripol	1915.00		NIST Webbook
ripol	1930.00		NIST Webbook
ripol	1959.00		NIST Webbook
ripol	1968.00		NIST Webbook
ripol	1958.00		NIST Webbook
ripol	1975.00		NIST Webbook
ripol	1978.00		NIST Webbook
tb	576.93	K	Joback Method
tc	782.93	K	Joback Method
tf	323.58	K	Joback Method
vc	0.624	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	394.04	J/mol×K	576.93	Joback Method
cpg	409.22	J/mol×K	611.26	Joback Method
cpg	423.55	J/mol×K	645.60	Joback Method
cpg	437.06	J/mol×K	679.93	Joback Method
cpg	449.76	J/mol×K	714.26	Joback Method
cpg	461.69	J/mol×K	748.60	Joback Method
cpg	472.86	J/mol×K	782.93	Joback Method
dvisc	0.0022442	Pa×s	323.58	Joback Method
dvisc	0.0011633	Pa×s	365.81	Joback Method
dvisc	0.0006908	Pa×s	408.03	Joback Method
dvisc	0.0004524	Pa×s	450.25	Joback Method
dvisc	0.0003185	Pa×s	492.48	Joback Method
dvisc	0.0002371	Pa×s	534.70	Joback Method
dvisc	0.0001842	Pa×s	576.93	Joback Method

hvapt	69.70	kJ/mol	298.15	Vapor pressures and vaporization enthalpies of a series of esters used in flavors by correlation gas chromatography

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C103526&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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