Octanoic acid, 2-phenylethyl ester

Other names:	Octanoic acid, phenethyl ester
	Phenylethyl octanoate
	2-Phenethyl octanoate
	2-Phenylethyl octanoate
	Phenethyl octanoate
	Phenylethyl n-octanoate
	2-Phenylethyl-n-octanoate
	Octanoic acid phenylethyl ester
Inchi:	InChI=1S/C16H24O2/c1-2-3-4-5-9-12-16(17)18-14-13-15-10-7-6-8-11-15/h6-8,10-11H,2-
InchiKey:	ASETYIALRXDVDF-UHFFFAOYSA-N
Formula:	C16H24O2
SMILES:	CCCCCCCC(=O)OCCc1ccccc1
Mol. weight [g/mol]:	248.36
CAS:	5457-70-5

Physical Properties

Property code	Value	Unit	Source
gf	-37.67	kJ/mol	Joback Method
hf	-381.84	kJ/mol	Joback Method
hfus	34.02	kJ/mol	Joback Method
hvap	62.64	kJ/mol	Joback Method
log10ws	-4.49		Crippen Method
logp	4.133		Crippen Method
mcvol	219.980	ml/mol	McGowan Method
pc	1769.87	kPa	Joback Method
rinpol	1846.00		NIST Webbook
rinpol	1857.00		NIST Webbook
rinpol	1842.00		NIST Webbook
rinpol	1864.00		NIST Webbook
rinpol	1809.00		NIST Webbook
rinpol	1819.00		NIST Webbook
rinpol	1854.40		NIST Webbook
rinpol	1820.00		NIST Webbook
rinpol	1846.00		NIST Webbook
rinpol	1819.00		NIST Webbook
rinpol	1847.00		NIST Webbook
rinpol	1814.00		NIST Webbook

rinpol	1838.00		NIST Webbook
rinpol	1854.40		NIST Webbook
rinpol	1820.00		NIST Webbook
rinpol	1856.00		NIST Webbook
rinpol	1838.00		NIST Webbook
ripol	2337.00		NIST Webbook
ripol	2373.00		NIST Webbook
ripol	2376.00		NIST Webbook
ripol	2335.00		NIST Webbook
ripol	2373.00		NIST Webbook
ripol	2376.00		NIST Webbook
ripol	2335.00		NIST Webbook
tb	668.45	K	Joback Method
tc	863.72	K	Joback Method
tf	368.66	K	Joback Method
vc	0.848	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	599.99	J/mol×K	668.45	Joback Method
cpg	617.16	J/mol×K	701.00	Joback Method
cpg	633.37	J/mol×K	733.54	Joback Method
cpg	648.65	J/mol×K	766.09	Joback Method
cpg	663.03	J/mol×K	798.63	Joback Method
cpg	676.54	J/mol×K	831.18	Joback Method
cpg	689.21	J/mol×K	863.72	Joback Method
dvisc	0.0018111	Pa×s	368.66	Joback Method
dvisc	0.0008831	Pa×s	418.62	Joback Method
dvisc	0.0005018	Pa×s	468.59	Joback Method
dvisc	0.0003180	Pa×s	518.55	Joback Method
dvisc	0.0002183	Pa×s	568.52	Joback Method
dvisc	0.0001593	Pa×s	618.48	Joback Method
dvisc	0.0001218	Pa×s	668.45	Joback Method

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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=C5457705&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
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