PHENETHYL OCTANOATE

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]:	248.37

Physical Properties

Property code	Value	Unit	Source
af	0.7518		Cheméo Relay (1.0)
gf	-37.67	kJ/mol	Joback Method
hf	-438.53	kJ/mol	Cheméo Relay (1.0)
hfus	34.02	kJ/mol	Joback Method
hvap	82.85	kJ/mol	Cheméo Relay (1.0)
ie	8.70	eV	Cheméo Relay (1.0)
log10ws	-4.71		Cheméo Relay (1.0)
logp	4.133		Crippen Method
mcvol	219.980	ml/mol	McGowan Method
pc	1769.87	kPa	Joback Method
rinpol	1857.00		NIST Webbook
rinpol	1864.00		NIST Webbook
rinpol	1819.00		NIST Webbook
rinpol	1846.00		NIST Webbook
rinpol	1838.00		NIST Webbook
rinpol	1820.00		NIST Webbook
rinpol	1819.00		NIST Webbook
rinpol	1856.00		NIST Webbook
rinpol	1842.00		NIST Webbook
rinpol	1854.40		NIST Webbook
rinpol	1820.00		NIST Webbook

rinpol	1854.40		NIST Webbook
rinpol	1838.00		NIST Webbook
rinpol	1814.00		NIST Webbook
rinpol	1847.00		NIST Webbook
rinpol	1809.00		NIST Webbook
rinpol	1846.00		NIST Webbook
ripol	2373.00		NIST Webbook
ripol	2376.00		NIST Webbook
ripol	2335.00		NIST Webbook
ripol	2337.00		NIST Webbook
ripol	2373.00		NIST Webbook
ripol	2376.00		NIST Webbook
ripol	2335.00		NIST Webbook
tb	587.81	K	Cheméo Relay (1.0)
tc	782.22	K	Cheméo Relay (1.0)
tf	255.07	K	Cheméo Relay (1.0)
vc	0.828	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

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

Sources

Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5457705&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	

Legend

af:	Acentric Factor
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
ie:	Ionization energy
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