2-Phenoxyethyl pentanoate

Inchi: InChI=1S/C13H18O3/c1-2-3-9-13(14)16-11-10-15-12-7-5-4-6-8-12/h4-8H,2-3,9-11H2,1H
InchiKey: VTDVFBXXQCGSIB-UHFFFAOYSA-N
Formula: C13H18O3
SMILES: CCCCC(=O)OCCOc1ccccc1
Mol. weight [g/mol]: 222.28

Physical Properties

Property code	Value	Unit	Source
gf	-167.93	kJ/mol	Joback Method
hf	-452.14	kJ/mol	Joback Method
hfus	27.44	kJ/mol	Joback Method
hvap	58.37	kJ/mol	Joback Method
log10ws	-2.97		Crippen Method
logp	2.799		Crippen Method
mcvol	183.580	ml/mol	McGowan Method
pc	2254.67	kPa	Joback Method
rinpol	1619.00		NIST Webbook
tb	622.23	K	Joback Method
tc	823.28	K	Joback Method
tf	357.08	K	Joback Method
vc	0.698	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	469.84	J/mol×K	622.23	Joback Method
cpg	538.87	J/mol×K	789.77	Joback Method
cpg	526.70	J/mol×K	756.26	Joback Method
cpg	513.73	J/mol×K	722.75	Joback Method
cpg	499.93	J/mol×K	689.25	Joback Method
cpg	485.31	J/mol×K	655.74	Joback Method
cpg	550.25	J/mol×K	823.28	Joback Method
dvisc	0.0001331	Pa×s	622.23	Joback Method
dvisc	0.0001715	Pa×s	578.04	Joback Method

dvisc	0.0002302	Pa×s	533.85	Joback Method
dvisc	0.0003261	Pa×s	489.66	Joback Method
dvisc	0.0004948	Pa×s	445.46	Joback Method
dvisc	0.0008230	Pa×s	401.27	Joback Method
dvisc	0.0015527	Pa×s	357.08	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R540871&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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