2-Phenoxyethyl caprylate

Inchi: InChI=1S/C16H24O3/c1-2-3-4-5-9-12-16(17)19-14-13-18-15-10-7-6-8-11-15/h6-8,10-11H
InchiKey: FTLLYZOWBWEERE-UHFFFAOYSA-N
Formula: C16H24O3
SMILES: CCCCCCCC(=O)OCCOc1ccccc1
Mol. weight [g/mol]: 264.36

Physical Properties

Property code	Value	Unit	Source
gf	-142.67	kJ/mol	Joback Method
hf	-514.06	kJ/mol	Joback Method
hfus	35.21	kJ/mol	Joback Method
hvap	65.05	kJ/mol	Joback Method
log10ws	-4.22		Crippen Method
logp	3.969		Crippen Method
mcvol	225.850	ml/mol	McGowan Method
pc	1744.82	kPa	Joback Method
rinpol	1916.00		NIST Webbook
rinpol	1916.00		NIST Webbook
tb	690.87	K	Joback Method
tc	885.06	K	Joback Method
tf	390.89	K	Joback Method
vc	0.866	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	628.67	J/mol×K	690.87	Joback Method
cpg	703.35	J/mol×K	852.69	Joback Method
cpg	690.23	J/mol×K	820.33	Joback Method
cpg	676.22	J/mol×K	787.96	Joback Method
cpg	661.30	J/mol×K	755.60	Joback Method
cpg	645.46	J/mol×K	723.23	Joback Method
cpg	715.59	J/mol×K	885.06	Joback Method
dvisc	0.0000944	Pa×s	690.87	Joback Method

dvisc	0.0001230	Pa×s	640.87	Joback Method
dvisc	0.0001676	Pa×s	590.88	Joback Method
dvisc	0.0002417	Pa×s	540.88	Joback Method
dvisc	0.0003755	Pa×s	490.88	Joback Method
dvisc	0.0006449	Pa×s	440.89	Joback Method
dvisc	0.0012718	Pa×s	390.89	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R540811&Units=SI

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