2-Phenoxyethyl caprate

Inchi: InChI=1S/C18H28O3/c1-2-3-4-5-6-7-11-14-18(19)21-16-15-20-17-12-9-8-10-13-17/h8-10
InchiKey: JBVZCOPEBAWJOB-UHFFFAOYSA-N
Formula: C18H28O3
SMILES: CCCCCCCCCC(=O)OCCOc1ccccc1
Mol. weight [g/mol]: 292.41

Physical Properties

Property code	Value	Unit	Source
gf	-125.83	kJ/mol	Joback Method
hf	-555.34	kJ/mol	Joback Method
hfus	40.39	kJ/mol	Joback Method
hvap	69.50	kJ/mol	Joback Method
log10ws	-5.06		Crippen Method
logp	4.749		Crippen Method
mcvol	254.030	ml/mol	McGowan Method
pc	1495.35	kPa	Joback Method
rinpol	2118.00		NIST Webbook
rinpol	2118.00		NIST Webbook
tb	736.63	K	Joback Method
tc	928.27	K	Joback Method
tf	413.43	K	Joback Method
vc	0.978	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	740.74	J/mol×K	736.63	Joback Method
cpg	758.14	J/mol×K	768.57	Joback Method
cpg	774.52	J/mol×K	800.51	Joback Method
cpg	789.93	J/mol×K	832.45	Joback Method
cpg	804.37	J/mol×K	864.39	Joback Method
cpg	817.87	J/mol×K	896.33	Joback Method
cpg	830.45	J/mol×K	928.27	Joback Method
dvisc	0.0010750	Pa×s	413.43	Joback Method

dvisc	0.0005311	Pa×s	467.30	Joback Method
dvisc	0.0003035	Pa×s	521.16	Joback Method
dvisc	0.0001927	Pa×s	575.03	Joback Method
dvisc	0.0001322	Pa×s	628.90	Joback Method
dvisc	0.0000962	Pa×s	682.76	Joback Method
dvisc	0.0000734	Pa×s	736.63	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=R540797&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