2-Hydroxyethyl heptadecanoate

Inchi: InChI=1S/C19H38O3/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-19(21)22-18-17-20/h20H
InchiKey: VGDYDZQOBOBURK-UHFFFAOYSA-N
Formula: C19H38O3
SMILES: CCCCCCCCCCCCCCCCC(=O)OCCO
Mol. weight [g/mol]: 314.50

Physical Properties

Property code	Value	Unit	Source
gf	-261.64	kJ/mol	Joback Method
hf	-832.52	kJ/mol	Joback Method
hfus	51.84	kJ/mol	Joback Method
hvap	83.72	kJ/mol	Joback Method
log10ws	-5.90		Crippen Method
logp	5.393		Crippen Method
mcvol	291.880	ml/mol	McGowan Method
pc	1185.79	kPa	Joback Method
rinpol	2326.00		NIST Webbook
rinpol	2326.00		NIST Webbook
tb	802.59	K	Joback Method
tc	982.99	K	Joback Method
tf	436.87	K	Joback Method
vc	1.143	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	926.26	J/mol×K	802.59	Joback Method
cpg	943.86	J/mol×K	832.66	Joback Method
cpg	960.54	J/mol×K	862.72	Joback Method
cpg	976.33	J/mol×K	892.79	Joback Method
cpg	991.25	J/mol×K	922.86	Joback Method
cpg	1005.33	J/mol×K	952.93	Joback Method
cpg	1018.60	J/mol×K	982.99	Joback Method
dvisc	0.0011580	Pa×s	436.87	Joback Method

dvisc	0.0003581	Pa×s	497.82	Joback Method
dvisc	0.0001431	Pa×s	558.78	Joback Method
dvisc	0.0000685	Pa×s	619.73	Joback Method
dvisc	0.0000374	Pa×s	680.68	Joback Method
dvisc	0.0000225	Pa×s	741.64	Joback Method
dvisc	0.0000147	Pa×s	802.59	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=R540480&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume