2-Hydroxyethyl nonadeanoate

Inchi: InChI=1S/C21H42O3/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-21(23)24-20-19-22
InchiKey: NFJKNKPGOUEIRS-UHFFFAOYSA-N
Formula: C21H42O3
SMILES: CCCCCCCCCCCCCCCCCCC(=O)OCCO
Mol. weight [g/mol]: 342.56

Physical Properties

Property code	Value	Unit	Source
gf	-244.80	kJ/mol	Joback Method
hf	-873.80	kJ/mol	Joback Method
hfus	57.02	kJ/mol	Joback Method
hvap	88.17	kJ/mol	Joback Method
log10ws	-6.74		Crippen Method
logp	6.174		Crippen Method
mcvol	320.060	ml/mol	McGowan Method
pc	1043.27	kPa	Joback Method
rinpol	2555.00		NIST Webbook
tb	848.35	K	Joback Method
tc	1039.11	K	Joback Method
tf	459.41	K	Joback Method
vc	1.254	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1048.28	J/mol×K	848.35	Joback Method
cpg	1067.15	J/mol×K	880.14	Joback Method
cpg	1084.95	J/mol×K	911.94	Joback Method
cpg	1101.71	J/mol×K	943.73	Joback Method
cpg	1117.46	J/mol×K	975.52	Joback Method
cpg	1132.25	J/mol×K	1007.31	Joback Method
cpg	1146.10	J/mol×K	1039.11	Joback Method
dvisc	0.0007975	Pa×s	459.41	Joback Method
dvisc	0.0002456	Pa×s	524.23	Joback Method

dvisc	0.0000980	Pa×s	589.06	Joback Method
dvisc	0.0000469	Pa×s	653.88	Joback Method
dvisc	0.0000257	Pa×s	718.70	Joback Method
dvisc	0.0000155	Pa×s	783.53	Joback Method
dvisc	0.0000101	Pa×s	848.35	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R540504&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