1,3-Propanediol, ethyl octacosyl ether

Inchi: InChI=1S/C33H68O2/c1-3-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-24-25
InchiKey: ATIZFDSCPHCBMK-UHFFFAOYSA-N
Formula: C33H68O2
SMILES: CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCOCCCOCC
Mol. weight [g/mol]: 496.89

Physical Properties

Property code	Value	Unit	Source
gf	16.98	kJ/mol	Joback Method
hf	-988.89	kJ/mol	Joback Method
hfus	83.60	kJ/mol	Joback Method
hvap	93.87	kJ/mol	Joback Method
log10ws	-11.81		Crippen Method
logp	11.592		Crippen Method
mcvol	487.570	ml/mol	McGowan Method
pc	511.87	kPa	Joback Method
rinpol	3357.00		NIST Webbook
rinpol	3357.00		NIST Webbook
tb	999.28	K	Joback Method
tc	1265.69	K	Joback Method
tf	506.13	K	Joback Method
vc	1.919	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1758.31	J/mol×K	999.28	Joback Method
cpg	1887.24	J/mol×K	1221.29	Joback Method
cpg	1866.39	J/mol×K	1176.89	Joback Method
cpg	1843.21	J/mol×K	1132.48	Joback Method
cpg	1817.57	J/mol×K	1088.08	Joback Method
cpg	1789.31	J/mol×K	1043.68	Joback Method
cpg	1905.92	J/mol×K	1265.69	Joback Method
dvisc	0.0000082	Pa×s	999.28	Joback Method

dvisc	0.0000114	Pa×s	917.09	Joback Method
dvisc	0.0000169	Pa×s	834.90	Joback Method
dvisc	0.0000273	Pa×s	752.70	Joback Method
dvisc	0.0000496	Pa×s	670.51	Joback Method
dvisc	0.0001064	Pa×s	588.32	Joback Method
dvisc	0.0002924	Pa×s	506.13	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406359&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