1,3-Propanediol, ethyl triacontyl ether

Inchi: InChI=1S/C35H72O2/c1-3-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-24-25
InchiKey: TXXXKIKIOHIGPF-UHFFFAOYSA-N
Formula: C35H72O2
SMILES: CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCOCCCOCC
Mol. weight [g/mol]: 524.95

Physical Properties

Property code	Value	Unit	Source
gf	33.82	kJ/mol	Joback Method
hf	-1030.17	kJ/mol	Joback Method
hfus	88.78	kJ/mol	Joback Method
hvap	98.32	kJ/mol	Joback Method
log10ws	-12.65		Crippen Method
logp	12.372		Crippen Method
mcvol	515.750	ml/mol	McGowan Method
pc	470.13	kPa	Joback Method
rinpol	3554.00		NIST Webbook
rinpol	3554.00		NIST Webbook
tb	1045.04	K	Joback Method
tc	1347.40	K	Joback Method
tf	528.67	K	Joback Method
vc	2.031	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1895.30	J/mol×K	1045.04	Joback Method
cpg	2031.37	J/mol×K	1297.01	Joback Method
cpg	2010.22	J/mol×K	1246.61	Joback Method
cpg	1986.26	J/mol×K	1196.22	Joback Method
cpg	1959.28	J/mol×K	1145.83	Joback Method
cpg	1929.03	J/mol×K	1095.43	Joback Method
cpg	2049.94	J/mol×K	1347.40	Joback Method
dvisc	0.0000060	Pa×s	1045.04	Joback Method

dvisc	0.0000083	Pa×s	958.98	Joback Method
dvisc	0.0000123	Pa×s	872.92	Joback Method
dvisc	0.0000199	Pa×s	786.86	Joback Method
dvisc	0.0000364	Pa×s	700.79	Joback Method
dvisc	0.0000785	Pa×s	614.73	Joback Method
dvisc	0.0002176	Pa×s	528.67	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=U406360&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