1,3-Propanediol, ethyl dotriacontyl ether

Inchi: InChI=1S/C37H76O2/c1-3-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-24-25
InchiKey: OXRUMAJOYXFQNW-UHFFFAOYSA-N
Formula: C37H76O2
SMILES: CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCOCCCOCC
Mol. weight [g/mol]: 553.00

Physical Properties

Property code	Value	Unit	Source
gf	50.66	kJ/mol	Joback Method
hf	-1071.45	kJ/mol	Joback Method
hfus	93.96	kJ/mol	Joback Method
hvap	102.78	kJ/mol	Joback Method
log10ws	-13.48		Crippen Method
logp	13.152		Crippen Method
mcvol	543.930	ml/mol	McGowan Method
pc	433.31	kPa	Joback Method
rinpol	3751.00		NIST Webbook
tb	1090.80	K	Joback Method
tc	1437.49	K	Joback Method
tf	551.21	K	Joback Method
vc	2.143	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	2032.95	J/mol×K	1090.80	Joback Method
cpg	2069.78	J/mol×K	1148.58	Joback Method
cpg	2102.16	J/mol×K	1206.36	Joback Method
cpg	2130.46	J/mol×K	1264.15	Joback Method
cpg	2155.06	J/mol×K	1321.93	Joback Method
cpg	2176.32	J/mol×K	1379.71	Joback Method
cpg	2194.61	J/mol×K	1437.49	Joback Method
dvisc	0.0001609	Pa×s	551.21	Joback Method
dvisc	0.0000576	Pa×s	641.14	Joback Method

dvisc	0.0000265	Pa×s	731.07	Joback Method
dvisc	0.0000145	Pa×s	821.00	Joback Method
dvisc	0.0000089	Pa×s	910.94	Joback Method
dvisc	0.0000060	Pa×s	1000.87	Joback Method
dvisc	0.0000043	Pa×s	1090.80	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=U406361&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

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