1,3-Propanediol, eicosyl ethyl ether

Inchi: InChI=1S/C25H52O2/c1-3-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-23-27-25-22
InchiKey: RNICXQGWDRJREC-UHFFFAOYSA-N
Formula: C25H52O2
SMILES: CCCCCCCCCCCCCCCCCCCCCOCCCOCC
Mol. weight [g/mol]: 384.68

Physical Properties

Property code	Value	Unit	Source
gf	-50.38	kJ/mol	Joback Method
hf	-823.77	kJ/mol	Joback Method
hfus	62.88	kJ/mol	Joback Method
hvap	76.06	kJ/mol	Joback Method
log10ws	-8.46		Crippen Method
logp	8.471		Crippen Method
mcvol	374.850	ml/mol	McGowan Method
pc	749.79	kPa	Joback Method
rinpol	2571.00		NIST Webbook
rinpol	2571.00		NIST Webbook
tb	816.24	K	Joback Method
tc	999.55	K	Joback Method
tf	415.97	K	Joback Method
vc	1.472	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1223.45	J/mol×K	816.24	Joback Method
cpg	1246.86	J/mol×K	846.79	Joback Method
cpg	1269.02	J/mol×K	877.34	Joback Method
cpg	1289.97	J/mol×K	907.89	Joback Method
cpg	1309.74	J/mol×K	938.44	Joback Method
cpg	1328.36	J/mol×K	969.00	Joback Method
cpg	1345.85	J/mol×K	999.55	Joback Method
dvisc	0.0008725	Pa×s	415.97	Joback Method

dvisc	0.0003319	Pa×s	482.68	Joback Method
dvisc	0.0001597	Pa×s	549.39	Joback Method
dvisc	0.0000900	Pa×s	616.11	Joback Method
dvisc	0.0000568	Pa×s	682.82	Joback Method
dvisc	0.0000388	Pa×s	749.53	Joback Method
dvisc	0.0000283	Pa×s	816.24	Joback Method

Sources

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=U406355&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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