1,3-Propanediol, ethyl hexadecyl ether

Inchi: InChI=1S/C21H44O2/c1-3-5-6-7-8-9-10-11-12-13-14-15-16-17-19-23-21-18-20-22-4-2/h3
InchiKey: JHCSLWDHWPAAFF-UHFFFAOYSA-N
Formula: C21H44O2
SMILES: CCCCCCCCCCCCCCCCOCCCOCC
Mol. weight [g/mol]: 328.57

Physical Properties

Property code	Value	Unit	Source
gf	-84.06	kJ/mol	Joback Method
hf	-741.21	kJ/mol	Joback Method
hfus	52.52	kJ/mol	Joback Method
hvap	67.16	kJ/mol	Joback Method
log10ws	-6.79		Crippen Method
logp	6.911		Crippen Method
mcvol	318.490	ml/mol	McGowan Method
pc	936.35	kPa	Joback Method
rinpol	2176.00		NIST Webbook
rinpol	2176.00		NIST Webbook
tb	724.72	K	Joback Method
tc	891.40	K	Joback Method
tf	370.89	K	Joback Method
vc	1.248	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	970.02	J/mol×K	724.72	Joback Method
cpg	1066.31	J/mol×K	863.62	Joback Method
cpg	1048.86	J/mol×K	835.84	Joback Method
cpg	1030.52	J/mol×K	808.06	Joback Method
cpg	1011.27	J/mol×K	780.28	Joback Method
cpg	991.12	J/mol×K	752.50	Joback Method
cpg	1082.90	J/mol×K	891.40	Joback Method
dvisc	0.0000500	Pa×s	724.72	Joback Method

dvisc	0.0000681	Pa×s	665.75	Joback Method
dvisc	0.0000985	Pa×s	606.78	Joback Method
dvisc	0.0001544	Pa×s	547.81	Joback Method
dvisc	0.0002696	Pa×s	488.83	Joback Method
dvisc	0.0005487	Pa×s	429.86	Joback Method
dvisc	0.0013998	Pa×s	370.89	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=U406353&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