1,3-Propanediol, dodecyl ethyl ether

Inchi: InChI=1S/C17H36O2/c1-3-5-6-7-8-9-10-11-12-13-15-19-17-14-16-18-4-2/h3-17H2,1-2H3
InchiKey: NLZDJFKXQXLTAF-UHFFFAOYSA-N
Formula: C17H36O2
SMILES: CCCCCCCCCCCCOCCCOCC
Mol. weight [g/mol]: 272.47

Physical Properties

Property code	Value	Unit	Source
gf	-117.74	kJ/mol	Joback Method
hf	-658.65	kJ/mol	Joback Method
hfus	42.16	kJ/mol	Joback Method
hvap	58.26	kJ/mol	Joback Method
log10ws	-5.11		Crippen Method
logp	5.350		Crippen Method
mcvol	262.130	ml/mol	McGowan Method
pc	1202.29	kPa	Joback Method
rinpol	1780.00		NIST Webbook
rinpol	1780.00		NIST Webbook
tb	633.20	K	Joback Method
tc	793.50	K	Joback Method
tf	325.81	K	Joback Method
vc	1.024	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	731.90	J/mol×K	633.20	Joback Method
cpg	820.33	J/mol×K	766.78	Joback Method
cpg	804.09	J/mol×K	740.07	Joback Method
cpg	787.13	J/mol×K	713.35	Joback Method
cpg	769.45	J/mol×K	686.63	Joback Method
cpg	751.05	J/mol×K	659.92	Joback Method
cpg	835.88	J/mol×K	793.50	Joback Method
dvisc	0.0000839	Pa×s	633.20	Joback Method

dvisc	0.0001132	Pa×s	581.97	Joback Method
dvisc	0.0001619	Pa×s	530.74	Joback Method
dvisc	0.0002499	Pa×s	479.50	Joback Method
dvisc	0.0004278	Pa×s	428.27	Joback Method
dvisc	0.0008477	Pa×s	377.04	Joback Method
dvisc	0.0020826	Pa×s	325.81	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406351&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