

1,3-Propanediol, ethyl tetradecyl ether

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C19H40O2/c1-3-5-6-7-8-9-10-11-12-13-14-15-17-21-19-16-18-20-4-2/h3-19H2

WCQUANOJDBCKLD-UHFFFAOYSA-N

C19H40O2

CCCCCCCCCCCCCOCCCOCC

300.52

Physical Properties

Property code	Value	Unit	Source
gf	-100.90	kJ/mol	Joback Method
hf	-699.93	kJ/mol	Joback Method
hfus	47.34	kJ/mol	Joback Method
hvap	62.71	kJ/mol	Joback Method
log10ws	-5.95		Crippen Method
logp	6.131		Crippen Method
mcvol	290.310	ml/mol	McGowan Method
pc	1056.88	kPa	Joback Method
rinpol	1976.00		NIST Webbook
rinpol	1976.00		NIST Webbook
tb	678.96	K	Joback Method
tc	841.42	K	Joback Method
tf	348.35	K	Joback Method
vc	1.135	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	848.72	J/mol×K	678.96	Joback Method
cpg	868.83	J/mol×K	706.04	Joback Method
cpg	888.12	J/mol×K	733.11	Joback Method
cpg	906.59	J/mol×K	760.19	Joback Method
cpg	924.25	J/mol×K	787.26	Joback Method
cpg	941.13	J/mol×K	814.34	Joback Method
cpg	957.23	J/mol×K	841.42	Joback Method
dvisc	0.0017266	Pa×s	348.35	Joback Method

dvisc	0.0006889	Pa×s	403.45	Joback Method
dvisc	0.0003428	Pa×s	458.55	Joback Method
dvisc	0.0001981	Pa×s	513.65	Joback Method
dvisc	0.0001273	Pa×s	568.76	Joback Method
dvisc	0.0000885	Pa×s	623.86	Joback Method
dvisc	0.0000652	Pa×s	678.96	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406352&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cp_g:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
g_f:	Standard Gibbs free energy of formation
h_f:	Enthalpy of formation at standard conditions
h_{fus}:	Enthalpy of fusion at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
log_{10ws}:	Log10 of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mc_{vol}:	McGowan's characteristic volume
p_c:	Critical Pressure
rin_{pol}:	Non-polar retention indices
t_b:	Normal Boiling Point Temperature
t_c:	Critical Temperature
t_f:	Normal melting (fusion) point
v_c:	Critical Volume

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