

1,3-Propanediol, decyl ethyl ether

Inchi:	InChI=1S/C15H32O2/c1-3-5-6-7-8-9-10-11-13-17-15-12-14-16-4-2/h3-15H2,1-2H3
InchiKey:	JPCNMBFSVIQKFK-UHFFFAOYSA-N
Formula:	C15H32O2
SMILES:	CCCCCCCCCOCCCOCC
Mol. weight [g/mol]:	244.41

Physical Properties

Property code	Value	Unit	Source
gf	-134.58	kJ/mol	Joback Method
hf	-617.37	kJ/mol	Joback Method
hfus	36.98	kJ/mol	Joback Method
hvap	53.80	kJ/mol	Joback Method
log10ws	-4.28		Crippen Method
logp	4.570		Crippen Method
mvol	233.950	ml/mol	McGowan Method
pc	1379.91	kPa	Joback Method
rinpol	1585.00		NIST Webbook
rinpol	1585.00		NIST Webbook
tb	587.44	K	Joback Method
tc	747.21	K	Joback Method
tf	303.27	K	Joback Method
vc	0.911	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	620.29	J/molxK	587.44	Joback Method
cpg	638.39	J/molxK	614.07	Joback Method
cpg	655.83	J/molxK	640.70	Joback Method
cpg	672.63	J/molxK	667.32	Joback Method
cpg	688.78	J/molxK	693.95	Joback Method
cpg	704.29	J/molxK	720.58	Joback Method
cpg	719.16	J/molxK	747.21	Joback Method
dvisc	0.0024441	Paxs	303.27	Joback Method

dvisc	0.0010177	Paxs	350.63	Joback Method
dvisc	0.0005220	Paxs	397.99	Joback Method
dvisc	0.0003086	Paxs	445.36	Joback Method
dvisc	0.0002019	Paxs	492.72	Joback Method
dvisc	0.0001422	Paxs	540.08	Joback Method
dvisc	0.0001060	Paxs	587.44	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U406350&Units=SI

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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