

1,3-Propanediol, ethyl hexacosyl ether

Inchi:	InChI=1S/C31H64O2/c1-3-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-24-25
InchiKey:	JYFLQDVUVLULNX-UHFFFAOYSA-N
Formula:	C31H64O2
SMILES:	CCCCCCCCCCCCCCCCCCCCCCCCCCOCCOCC
Mol. weight [g/mol]:	468.84

Physical Properties

Property code	Value	Unit	Source
gf	0.14	kJ/mol	Joback Method
hf	-947.61	kJ/mol	Joback Method
hfus	78.42	kJ/mol	Joback Method
hvap	89.42	kJ/mol	Joback Method
log10ws	-10.97		Crippen Method
logp	10.812		Crippen Method
mvol	459.390	ml/mol	McGowan Method
pc	559.41	kPa	Joback Method
rinpol	3163.00		NIST Webbook
rinpol	3163.00		NIST Webbook
tb	953.52	K	Joback Method
tc	1191.04	K	Joback Method
tf	483.59	K	Joback Method
vc	1.808	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1622.26	J/molxK	953.52	Joback Method
cpg	1744.37	J/molxK	1151.46	Joback Method
cpg	1723.97	J/molxK	1111.87	Joback Method
cpg	1701.66	J/molxK	1072.28	Joback Method
cpg	1677.33	J/molxK	1032.69	Joback Method
cpg	1650.89	J/molxK	993.11	Joback Method
cpg	1762.93	J/molxK	1191.04	Joback Method
dvisc	0.0000113	Paxs	953.52	Joback Method

dvisc	0.0000157	Paxs	875.20	Joback Method
dvisc	0.0000231	Paxs	796.88	Joback Method
dvisc	0.0000372	Paxs	718.56	Joback Method
dvisc	0.0000672	Paxs	640.23	Joback Method
dvisc	0.0001432	Paxs	561.91	Joback Method
dvisc	0.0003898	Paxs	483.59	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=U406358&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cp_g:	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:	Log ₁₀ 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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