

Isobutyl octacosyl ether

Inchi: InChI=1S/C32H66O/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-24-25-26-27-28-29-30-31-32
InchiKey: TYNVUCGWZAJDCT-UHFFFAOYSA-N
Formula: C32H66O
SMILES: CCCCCCCCCCCCCCCCCCCCCCCCCCCCCOCC(C)C
Mol. weight [g/mol]: 466.87

Physical Properties

Property code	Value	Unit	Source
gf	111.12	kJ/mol	Joback Method
hf	-841.31	kJ/mol	Joback Method
hfus	76.30	kJ/mol	Joback Method
hvap	88.85	kJ/mol	Joback Method
log10ws	-12.06		Crippen Method
logp	11.822		Crippen Method
mvol	467.610	ml/mol	McGowan Method
pc	541.08	kPa	Joback Method
rinpol	3223.00		NIST Webbook
rinpol	3223.00		NIST Webbook
tb	953.54	K	Joback Method
tc	1189.14	K	Joback Method
tf	457.63	K	Joback Method
vc	1.839	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1654.77	J/molxK	953.54	Joback Method
cpg	1781.94	J/molxK	1149.87	Joback Method
cpg	1760.20	J/molxK	1110.61	Joback Method
cpg	1736.73	J/molxK	1071.34	Joback Method
cpg	1711.41	J/molxK	1032.07	Joback Method
cpg	1684.13	J/molxK	992.81	Joback Method
cpg	1802.06	J/molxK	1189.14	Joback Method
dvisc	0.0000120	Paxs	953.54	Joback Method

dvisc	0.0000170	Paxs	870.89	Joback Method
dvisc	0.0000258	Paxs	788.24	Joback Method
dvisc	0.0000433	Paxs	705.59	Joback Method
dvisc	0.0000834	Paxs	622.93	Joback Method
dvisc	0.0001962	Paxs	540.28	Joback Method
dvisc	0.0006286	Paxs	457.63	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406334&Units=SI
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

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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