

Isobutyl tetratriacontyl ether

Inchi: InChI=1S/C38H78O/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-24-25-26-27-28-29-30-31-32-33-34-35-36-37-38
InchiKey: RRTKOWOOFOPUHY-UHFFFAOYSA-N
Formula: C38H78O
SMILES: CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCOCC(C)C
Mol. weight [g/mol]: 551.03

Physical Properties

Property code	Value	Unit	Source
gf	161.64	kJ/mol	Joback Method
hf	-965.15	kJ/mol	Joback Method
hfus	91.84	kJ/mol	Joback Method
hvap	102.20	kJ/mol	Joback Method
log10ws	-14.57		Crippen Method
logp	14.162		Crippen Method
mvol	552.150	ml/mol	McGowan Method
pc	420.78	kPa	Joback Method
rinpol	3826.00		NIST Webbook
rinpol	3826.00		NIST Webbook
tb	1090.82	K	Joback Method
tc	1432.84	K	Joback Method
tf	525.25	K	Joback Method
vc	2.175	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	2069.20	J/molxK	1090.82	Joback Method
cpg	2107.59	J/molxK	1147.82	Joback Method
cpg	2142.04	J/molxK	1204.83	Joback Method
cpg	2172.96	J/molxK	1261.83	Joback Method
cpg	2200.79	J/molxK	1318.83	Joback Method
cpg	2225.96	J/molxK	1375.84	Joback Method
cpg	2248.90	J/molxK	1432.84	Joback Method
dvisc	0.0002474	Paxs	525.25	Joback Method

dvisc	0.0000766	Paxs	619.51	Joback Method
dvisc	0.0000323	Paxs	713.77	Joback Method
dvisc	0.0000167	Paxs	808.03	Joback Method
dvisc	0.0000099	Paxs	902.30	Joback Method
dvisc	0.0000065	Paxs	996.56	Joback Method
dvisc	0.0000045	Paxs	1090.82	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406337&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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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