

3,3-Dimethylbutyl tert-octyl ether

Inchi:	InChI=1S/C14H30O/c1-12(2,3)9-10-15-14(7,8)11-13(4,5)6/h9-11H2,1-8H3
InchiKey:	CFYGAKVQHADXFE-UHFFFAOYSA-N
Formula:	C14H30O
SMILES:	CC(C)(C)CCOC(C)(C)CC(C)(C)C
Mol. weight [g/mol]:	214.39

Physical Properties

Property code	Value	Unit	Source
gf	-29.48	kJ/mol	Joback Method
hf	-490.76	kJ/mol	Joback Method
hfus	10.96	kJ/mol	Joback Method
hvap	45.28	kJ/mol	Joback Method
log10ws	-4.40		Crippen Method
logp	4.654		Crippen Method
mcvol	213.990	ml/mol	McGowan Method
pc	1572.21	kPa	Joback Method
rinsol	1221.00		NIST Webbook
tb	532.45	K	Joback Method
tc	718.97	K	Joback Method
tf	277.03	K	Joback Method
vc	0.804	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	543.73	J/molxK	532.45	Joback Method
cpg	564.92	J/molxK	563.54	Joback Method
cpg	584.92	J/molxK	594.62	Joback Method
cpg	603.81	J/molxK	625.71	Joback Method
cpg	621.64	J/molxK	656.80	Joback Method
cpg	638.47	J/molxK	687.88	Joback Method
cpg	654.35	J/molxK	718.97	Joback Method
dvisc	0.0088835	Paxs	277.03	Joback Method
dvisc	0.0027060	Paxs	319.60	Joback Method

dvisc	0.0010900	Paxs	362.17	Joback Method
dvisc	0.0005316	Paxs	404.74	Joback Method
dvisc	0.0002972	Paxs	447.31	Joback Method
dvisc	0.0001839	Paxs	489.88	Joback Method
dvisc	0.0001228	Paxs	532.45	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R559632&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

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
mccvol:	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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