

3-Methylpentyl tert-octyl ether

Inchi:	InChI=1S/C14H30O/c1-8-12(2)9-10-15-14(6,7)11-13(3,4)5/h12H,8-11H2,1-7H3
InchiKey:	XDHWZRZJHGHTKAG-UHFFFAOYSA-N
Formula:	C14H30O
SMILES:	CCC(C)CCOC(C)(C)CC(C)(C)C
Mol. weight [g/mol]:	214.39

Physical Properties

Property code	Value	Unit	Source
gf	-34.76	kJ/mol	Joback Method
hf	-487.29	kJ/mol	Joback Method
hfus	14.85	kJ/mol	Joback Method
hvap	46.19	kJ/mol	Joback Method
log10ws	-4.40		Crippen Method
logp	4.654		Crippen Method
mcvol	213.990	ml/mol	McGowan Method
pc	1558.58	kPa	Joback Method
rinpol	1266.00		NIST Webbook
tb	535.24	K	Joback Method
tc	715.21	K	Joback Method
tf	259.61	K	Joback Method
vc	0.809	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	541.49	J/molxK	535.24	Joback Method
cpg	633.55	J/molxK	685.21	Joback Method
cpg	616.99	J/molxK	655.22	Joback Method
cpg	599.55	J/molxK	625.22	Joback Method
cpg	581.18	J/molxK	595.23	Joback Method
cpg	561.84	J/molxK	565.23	Joback Method
cpg	649.25	J/molxK	715.21	Joback Method
dvisc	0.0001225	Paxs	535.24	Joback Method
dvisc	0.0001823	Paxs	489.30	Joback Method

dvisc	0.0002949	Paxs	443.36	Joback Method
dvisc	0.0005329	Paxs	397.43	Joback Method
dvisc	0.0011240	Paxs	351.49	Joback Method
dvisc	0.0029676	Paxs	305.55	Joback Method
dvisc	0.0110472	Paxs	259.61	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R559647&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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