4-Methylpentyl tert-octyl ether

Inchi: InChI=1S/C14H30O/c1-12(2)9-8-10-15-14(6,7)11-13(3,4)5/h12H,8-11H2,1-7H3
InchiKey: UUBSLYFKXOFLCA-UHFFFAOYSA-N
Formula: C14H30O
SMILES: CC(C)CCCOC(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	1252.00		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/mol×K	535.24	Joback Method
cpg	561.84	J/mol×K	565.23	Joback Method
cpg	581.18	J/mol×K	595.23	Joback Method
cpg	599.55	J/mol×K	625.22	Joback Method
cpg	616.99	J/mol×K	655.22	Joback Method
cpg	633.55	J/mol×K	685.21	Joback Method
cpg	649.25	J/mol×K	715.21	Joback Method
dvisc	0.0110472	Pa×s	259.61	Joback Method
dvisc	0.0029676	Pa×s	305.55	Joback Method

dvisc	0.0011240	Pa×s	351.49	Joback Method
dvisc	0.0005329	Pa×s	397.43	Joback Method
dvisc	0.0002949	Pa×s	443.36	Joback Method
dvisc	0.0001823	Pa×s	489.30	Joback Method
dvisc	0.0001225	Pa×s	535.24	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R559652&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
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