(R)-linden ether

Other names: linden ether
Inchi: InChI=1S/C10H14O/c1-7-3-4-9-8(2)6-11-10(9)5-7/h5,10H,3-4,6H2,1-2H3
InchiKey: NDGVBBGSPLJJRM-UHFFFAOYSA-N
Formula: C10H14O
SMILES: CC1=CC2OCC(C)=C2CC1
Mol. weight [g/mol]: 150.22
CAS: 125811-37-2

Physical Properties

Property code	Value	Unit	Source
gf	71.14	kJ/mol	Joback Method
hf	-153.12	kJ/mol	Joback Method
hfus	19.81	kJ/mol	Joback Method
hvap	45.59	kJ/mol	Joback Method
log10ws	-2.70		Crippen Method
logp	2.442		Crippen Method
mcvol	127.310	ml/mol	McGowan Method
pc	3114.04	kPa	Joback Method
rinpol	1235.00		NIST Webbook
rinpol	1235.00		NIST Webbook
rinpol	1252.00		NIST Webbook
rinpol	1252.00		NIST Webbook
tb	499.37	K	Joback Method
tc	720.11	K	Joback Method
tf	297.67	K	Joback Method
vc	0.479	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	289.58	J/mol×K	499.37	Joback Method
cpg	360.75	J/mol×K	683.32	Joback Method
cpg	348.28	J/mol×K	646.53	Joback Method
cpg	334.98	J/mol×K	609.74	Joback Method

cpg	320.79	J/mol×K	572.95	Joback Method
cpg	305.68	J/mol×K	536.16	Joback Method
cpg	372.44	J/mol×K	720.11	Joback Method
dvisc	0.0004492	Pa×s	499.37	Joback Method
dvisc	0.0005183	Pa×s	465.75	Joback Method
dvisc	0.0006115	Pa×s	432.14	Joback Method
dvisc	0.0007418	Pa×s	398.52	Joback Method
dvisc	0.0009326	Pa×s	364.90	Joback Method
dvisc	0.0012280	Pa×s	331.29	Joback Method
dvisc	0.0017208	Pa×s	297.67	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C125811372&Units=SI

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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