Diisobutylene oxide

Inchi: InChI=1S/2C8H16O/c1-7(2,3)6-8(4,5)9-6;1-7(2,3)5-8(4)6-9-8/h6H,1-5H3;5-6H2,1-4H3
InchiKey: YCLNWWLCPXGPLK-UHFFFAOYSA-N
Formula: C16H32O2
SMILES: CC(C)(C)C1OC1(C)C.CC(C)(C)CC1(C)CO1
Mol. weight [g/mol]: 256.42

Physical Properties

Property code	Value	Unit	Source
gf	-84.67	kJ/mol	Joback Method
hf	-610.95	kJ/mol	Joback Method
hfus	19.71	kJ/mol	Joback Method
hvap	55.15	kJ/mol	Joback Method
log10ws	-4.44		Crippen Method
logp	4.421		Crippen Method
mcvol	237.180	ml/mol	McGowan Method
pc	1593.62	kPa	Joback Method
tb	623.61	K	Joback Method
tc	840.19	K	Joback Method
tf	374.76	K	Joback Method
vc	0.878	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	683.61	J/mol×K	623.61	Joback Method
cpg	707.37	J/mol×K	659.71	Joback Method
cpg	729.81	J/mol×K	695.80	Joback Method
cpg	751.17	J/mol×K	731.90	Joback Method
cpg	771.69	J/mol×K	768.00	Joback Method
cpg	791.62	J/mol×K	804.10	Joback Method
cpg	811.19	J/mol×K	840.19	Joback Method

Sources

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=B6001291&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume