

2-(1,1-Dimethylethyl)-3-methyloxirene

Inchi:	InChI=1S/C7H12O/c1-5-6(8-5)7(2,3)4/h1-4H3
InchiKey:	WFKRADMNVAKTTM-UHFFFAOYSA-N
Formula:	C7H12O
SMILES:	CC1=C(C(C)(C)C)O1
Mol. weight [g/mol]:	112.17

Physical Properties

Property code	Value	Unit	Source
gf	3.94	kJ/mol	Joback Method
hf	-200.58	kJ/mol	Joback Method
hfus	11.96	kJ/mol	Joback Method
hvap	36.23	kJ/mol	Joback Method
log10ws	-2.34		Crippen Method
logp	2.294		Crippen Method
mcvol	100.200	ml/mol	McGowan Method
pc	3415.86	kPa	Joback Method
ripol	1246.00		NIST Webbook
ripol	1246.00		NIST Webbook
tb	403.81	K	Joback Method
tc	601.23	K	Joback Method
tf	245.62	K	Joback Method
vc	0.382	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	199.57	J/mol×K	403.81	Joback Method
cpg	211.68	J/mol×K	436.71	Joback Method
cpg	223.02	J/mol×K	469.62	Joback Method
cpg	233.62	J/mol×K	502.52	Joback Method
cpg	243.54	J/mol×K	535.42	Joback Method
cpg	252.82	J/mol×K	568.32	Joback Method
cpg	261.51	J/mol×K	601.23	Joback Method
dvisc	0.0019723	Paxs	245.62	Joback Method

dvisc	0.0013447	Paxs	271.99	Joback Method
dvisc	0.0009810	Paxs	298.35	Joback Method
dvisc	0.0007533	Paxs	324.72	Joback Method
dvisc	0.0006018	Paxs	351.08	Joback Method
dvisc	0.0004962	Paxs	377.44	Joback Method
dvisc	0.0004195	Paxs	403.81	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R633488&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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