2-Methylisoborneol

Inchi: InChI=1S/C11H20O/c1-9(2)8-5-6-10(9,3)11(4,12)7-8/h8,12H,5-7H2,1-4H3/t8?,10?,11-/m
InchiKey: LFYXNXGVLGKVCJ-BOBPJJCASA-N
Formula: C11H20O
SMILES: CC1(O)CC2CCC1(C)C2(C)C
Mol. weight [g/mol]: 168.28
CAS: 2371-42-8

Physical Properties

Property code	Value	Unit	Source
gf	-17.57	kJ/mol	Joback Method
hf	-278.12	kJ/mol	Joback Method
hfus	5.75	kJ/mol	Joback Method
hvap	52.69	kJ/mol	Joback Method
log10ws	-2.87		Crippen Method
logp	2.584		Crippen Method
mcvol	150.000	ml/mol	McGowan Method
pc	2992.59	kPa	Joback Method
rinpol	1164.00		NIST Webbook
rinpol	1164.00		NIST Webbook
rinpol	1210.00		NIST Webbook
rinpol	1158.00		NIST Webbook
rinpol	1158.00		NIST Webbook
rinpol	1204.00		NIST Webbook
rinpol	1180.00		NIST Webbook
rinpol	1201.00		NIST Webbook
rinpol	1197.00		NIST Webbook
rinpol	1210.00		NIST Webbook
rinpol	1188.00		NIST Webbook
rinpol	1183.00		NIST Webbook
ripol	1602.00		NIST Webbook
ripol	1562.00		NIST Webbook
ripol	1562.00		NIST Webbook
ripol	1592.00		NIST Webbook
ripol	1602.00		NIST Webbook
ripol	1599.00		NIST Webbook
ripol	1592.00		NIST Webbook
ripol	1592.00		NIST Webbook

ripol	1622.00		NIST Webbook
tb	552.39	K	Joback Method
tc	758.28	K	Joback Method
tf	370.13	K	Joback Method
vc	0.569	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	401.39	J/mol×K	552.39	Joback Method
cpg	417.57	J/mol×K	586.70	Joback Method
cpg	432.61	J/mol×K	621.02	Joback Method
cpg	446.78	J/mol×K	655.33	Joback Method
cpg	460.35	J/mol×K	689.65	Joback Method
cpg	473.60	J/mol×K	723.96	Joback Method
cpg	486.80	J/mol×K	758.28	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=C2371428&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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume