

1-Methylnorbornane

Inchi:	InChI=1S/C8H14/c1-8-4-2-7(6-8)3-5-8/h7H,2-6H2,1H3
InchiKey:	UTPHVTOEOCZQJU-UHFFFAOYSA-N
Formula:	C8H14
SMILES:	CC12CCC(CC1)C2
Mol. weight [g/mol]:	110.20
CAS:	10052-18-3

Physical Properties

Property code	Value	Unit	Source
chl	-5018.00 ± 1.00	kJ/mol	NIST Webbook
gf	120.39	kJ/mol	Joback Method
hf	-53.77	kJ/mol	Joback Method
hfl	-130.90 ± 1.10	kJ/mol	NIST Webbook
hfus	4.35	kJ/mol	Joback Method
hvap	32.25	kJ/mol	Joback Method
log10ws	-2.48		Crippen Method
logp	2.587		Crippen Method
mcvol	101.860	ml/mol	McGowan Method
pc	3646.53	kPa	Joback Method
tb	400.43	K	Joback Method
tc	611.15	K	Joback Method
tf	236.18	K	Joback Method
vc	0.388	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	200.59	J/mol×K	400.43	Joback Method
cpg	218.79	J/mol×K	435.55	Joback Method
cpg	235.46	J/mol×K	470.67	Joback Method
cpg	250.75	J/mol×K	505.79	Joback Method
cpg	264.80	J/mol×K	540.91	Joback Method
cpg	277.76	J/mol×K	576.03	Joback Method
cpg	289.76	J/mol×K	611.15	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C10052183&Units=SI
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

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase 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

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