

Bicyclo(2.2.1)heptan-2-ol, 2-methyl-, exo-

Inchi:	InChI=1S/C8H14O/c1-8(9)5-6-2-3-7(8)4-6/h6-7,9H,2-5H2,1H3/t6?,7?,8-/m1/s1
InchiKey:	QBAQBGVSOIIBKF-KAVNDROISA-N
Formula:	C8H14O
SMILES:	CC1(O)CC2CCC1C2
Mol. weight [g/mol]:	126.20
CAS:	3212-15-5

Physical Properties

Property code	Value	Unit	Source
gf	-24.14	kJ/mol	Joback Method
hf	-226.34	kJ/mol	Joback Method
hfus	9.51	kJ/mol	Joback Method
hvap	48.62	kJ/mol	Joback Method
log10ws	-1.85		Crippen Method
logp	1.557		Crippen Method
mcvol	107.730	ml/mol	McGowan Method
pc	3920.94	kPa	Joback Method
rinpol	998.00		NIST Webbook
rinpol	998.00		NIST Webbook
ripol	1471.00		NIST Webbook
ripol	1471.00		NIST Webbook
tb	487.94	K	Joback Method
tc	686.54	K	Joback Method
tf	292.76	K	Joback Method
vc	0.406	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	261.85	J/molxK	487.94	Joback Method
cpg	276.32	J/molxK	521.04	Joback Method
cpg	289.73	J/molxK	554.14	Joback Method
cpg	302.21	J/molxK	587.24	Joback Method
cpg	313.87	J/molxK	620.34	Joback Method

cpg	324.82	J/mol×K	653.44	Joback Method
cpg	335.18	J/mol×K	686.54	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=C3212155&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
rinpola:	Non-polar retention indices
ripola:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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