

Bicyclo[2.2.1]heptan-2-ol, 7,7-dimethyl, endo

Inchi:	InChI=1S/C9H16O/c1-9(2)6-3-4-7(9)8(10)5-6/h6-8,10H,3-5H2,1-2H3/t6-,7+,8-/m1/s1
InchiKey:	DELDHDFPNUZDOP-GJMOJQLCSA-N
Formula:	C9H16O
SMILES:	CC1(C)C2CCC1C(O)C2
Mol. weight [g/mol]:	140.22

Physical Properties

Property code	Value	Unit	Source
gf	-23.43	kJ/mol	Joback Method
hf	-267.32	kJ/mol	Joback Method
hfus	13.17	kJ/mol	Joback Method
hvap	50.54	kJ/mol	Joback Method
log10ws	-2.03		Crippen Method
logp	1.803		Crippen Method
mcvol	121.820	ml/mol	McGowan Method
pc	3356.75	kPa	Joback Method
ripol	1687.00		NIST Webbook
ripol	1687.00		NIST Webbook
tb	506.15	K	Joback Method
tc	701.94	K	Joback Method
tf	299.79	K	Joback Method
vc	0.461	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	307.80	J/molxK	506.15	Joback Method
cpg	323.32	J/molxK	538.78	Joback Method
cpg	337.82	J/molxK	571.41	Joback Method
cpg	351.42	J/molxK	604.04	Joback Method
cpg	364.21	J/molxK	636.67	Joback Method
cpg	376.31	J/molxK	669.30	Joback Method
cpg	387.81	J/molxK	701.94	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R99585&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
h vap:	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
ri pol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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