Bicyclo[2.2.2]octan-1-ol

Other names: 1-Hydroxybicyclo[2.2.2]octane
Inchi: InChI=1S/C8H14O/c9-8-4-1-7(2-5-8)3-6-8/h7,9H,1-6H2
InchiKey: UOTOQJFVJGLVGK-UHFFFAOYSA-N
Formula: C8H14O
SMILES: OC12CCC(CC1)CC2
Mol. weight [g/mol]: 126.20
CAS: 20534-58-1

Physical Properties

Property code	Value	Unit	Source
gf	-28.53	kJ/mol	Joback Method
hf	-212.16	kJ/mol	Joback Method
hfus	6.34	kJ/mol	Joback Method
hvap	49.10	kJ/mol	Joback Method
ie	9.65 ± 0.05	eV	NIST Webbook
log10ws	-2.09		Crippen Method
logp	1.701		Crippen Method
mcvol	107.730	ml/mol	McGowan Method
pc	4222.04	kPa	Joback Method
rinpol	1061.00		NIST Webbook
ripol	1598.00		NIST Webbook
tb	496.88	K	Joback Method
tc	703.22	K	Joback Method
tf	293.48	K	Joback Method
vc	0.399	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	260.76	J/mol×K	496.88	Joback Method
cpg	275.68	J/mol×K	531.27	Joback Method
cpg	289.48	J/mol×K	565.66	Joback Method
cpg	302.28	J/mol×K	600.05	Joback Method
cpg	314.21	J/mol×K	634.44	Joback Method

cpg	325.40	J/mol×K	668.83	Joback Method
cpg	335.98	J/mol×K	703.22	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C20534581&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.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
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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

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