Bicyclo[2.2.2]oct-5-ene-2-carbonitrile, (1«alpha»,2«alpha»,4«alpha»)-

Inchi: InChI=1S/C9H11N/c10-6-9-5-7-1-3-8(9)4-2-7/h1,3,7-9H,2,4-5H2/t7?,8?,9-/m1/s1
InchiKey: WFLYMJQGWKVLTO-AMDVSUOASA-N
Formula: C9H11N
SMILES: N#CC1CC2C=CC1CC2
Mol. weight [g/mol]: 133.19
CAS: 3008-14-8

Physical Properties

Property code	Value	Unit	Source
gf	277.63	kJ/mol	Joback Method
hf	151.00 ± 4.20	kJ/mol	NIST Webbook
hfus	14.93	kJ/mol	Joback Method
hvap	46.26	kJ/mol	Joback Method
log10ws	-2.37		Crippen Method
logp	2.112		Crippen Method
mcvol	113.030	ml/mol	McGowan Method
pc	3107.10	kPa	Joback Method
tb	523.91	K	Joback Method
tc	754.50	K	Joback Method
tf	281.54	K	Joback Method
vc	0.449	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	268.65	J/mol×K	523.91	Joback Method
cpg	283.97	J/mol×K	562.34	Joback Method
cpg	298.21	J/mol×K	600.77	Joback Method
cpg	311.42	J/mol×K	639.21	Joback Method
cpg	323.68	J/mol×K	677.64	Joback Method
cpg	335.06	J/mol×K	716.07	Joback Method
cpg	345.62	J/mol×K	754.50	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=C3008148&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume