2-chloro-2-cyano bicyclo[2.2.1]hept-5-ene, endo

Inchi: InChI=1S/C8H8ClN/c9-8(5-10)4-6-1-2-7(8)3-6/h1-2,6-7H,3-4H2
InchiKey: UCYKNDOOVFKJKU-UHFFFAOYSA-N
Formula: C8H8ClN
SMILES: N#CC1(Cl)CC2C=CC1C2
Mol. weight [g/mol]: 153.61

Physical Properties

Property code	Value	Unit	Source
gf	263.89	kJ/mol	Joback Method
hf	132.81	kJ/mol	Joback Method
hfus	12.34	kJ/mol	Joback Method
hvap	47.09	kJ/mol	Joback Method
log10ws	-2.46		Crippen Method
logp	2.084		Crippen Method
mcvol	111.180	ml/mol	McGowan Method
pc	3399.94	kPa	Joback Method
rinpol	1153.00		NIST Webbook
rinpol	1153.00		NIST Webbook
tb	534.43	K	Joback Method
tc	775.58	K	Joback Method
tf	327.61	K	Joback Method
vc	0.448	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	249.83	J/mol×K	534.43	Joback Method
cpg	261.84	J/mol×K	574.62	Joback Method
cpg	272.74	J/mol×K	614.81	Joback Method
cpg	282.72	J/mol×K	655.00	Joback Method
cpg	292.00	J/mol×K	695.20	Joback Method
cpg	300.77	J/mol×K	735.39	Joback Method
cpg	309.25	J/mol×K	775.58	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R417479&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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