2-Chlorobicyclo[2.2.1]hept-5-ene-exo-2-carboxam

Inchi: InChI=1S/C8H10ClNO/c9-8(7(10)11)4-5-1-2-6(8)3-5/h1-2,5-6H,3-4H2,(H2,10,11)
InchiKey: HPIILJFZJQHOSE-UHFFFAOYSA-N
Formula: C8H10ClNO
SMILES: NC(=O)C1(Cl)CC2C=CC1C2
Mol. weight [g/mol]: 171.62

Physical Properties

Property code	Value	Unit	Source
gf	68.24	kJ/mol	Joback Method
hf	-110.86	kJ/mol	Joback Method
hfus	17.63	kJ/mol	Joback Method
hvap	54.00	kJ/mol	Joback Method
log10ws	-1.81		Crippen Method
logp	1.045		Crippen Method
mcvol	121.350	ml/mol	McGowan Method
pc	4056.96	kPa	Joback Method
rinpol	1354.00		NIST Webbook
rinpol	1354.00		NIST Webbook
tb	558.75	K	Joback Method
tc	800.52	K	Joback Method
tf	395.81	K	Joback Method
vc	0.457	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	293.52	J/mol×K	558.75	Joback Method
cpg	306.59	J/mol×K	599.04	Joback Method
cpg	318.52	J/mol×K	639.34	Joback Method
cpg	329.54	J/mol×K	679.63	Joback Method
cpg	339.85	J/mol×K	719.93	Joback Method
cpg	349.66	J/mol×K	760.22	Joback Method
cpg	359.18	J/mol×K	800.52	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=R417499&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume