Adamantan-4-one, 1-chloro

Inchi: InChI=1S/C10H13ClO/c11-10-3-6-1-7(4-10)9(12)8(2-6)5-10/h6-8H,1-5H2
InchiKey: JPEOUSFBWXVGFX-UHFFFAOYSA-N
Formula: C10H13ClO
SMILES: O=C1C2CC3CC1CC(Cl)(C3)C2
Mol. weight [g/mol]: 184.66

Physical Properties

Property code	Value	Unit	Source
gf	55.75	kJ/mol	Joback Method
hf	-196.03	kJ/mol	Joback Method
hfus	12.44	kJ/mol	Joback Method
hvap	44.94	kJ/mol	Joback Method
log10ws	-2.51		Crippen Method
logp	2.373		Crippen Method
mcvol	132.990	ml/mol	McGowan Method
pc	3254.14	kPa	Joback Method
rinpol	1483.00		NIST Webbook
rinpol	1483.00		NIST Webbook
tb	553.51	K	Joback Method
tc	799.48	K	Joback Method
tf	370.56	K	Joback Method
vc	0.511	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	340.53	J/mol×K	553.51	Joback Method
cpg	358.68	J/mol×K	594.50	Joback Method
cpg	375.42	J/mol×K	635.50	Joback Method
cpg	390.97	J/mol×K	676.49	Joback Method
cpg	405.54	J/mol×K	717.49	Joback Method
cpg	419.37	J/mol×K	758.48	Joback Method
cpg	432.67	J/mol×K	799.48	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R44398&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
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