1-chloromethyladamantane

Inchi: InChI=1S/C11H17Cl/c12-7-11-4-8-1-9(5-11)3-10(2-8)6-11/h8-10H,1-7H2
InchiKey: VZUOFLCVOCPUCM-UHFFFAOYSA-N
Formula: C11H17Cl
SMILES: ClCC12CC3CC(CC(C3)C1)C2
Mol. weight [g/mol]: 184.71

Physical Properties

Property code	Value	Unit	Source
gf	186.76	kJ/mol	Joback Method
hf	-78.97	kJ/mol	Joback Method
hfus	15.52	kJ/mol	Joback Method
hvap	42.92	kJ/mol	Joback Method
log10ws	-3.30		Crippen Method
logp	3.442		Crippen Method
mcvol	145.510	ml/mol	McGowan Method
pc	2817.33	kPa	Joback Method
rinpol	1455.00		NIST Webbook
rinpol	1409.00		NIST Webbook
rinpol	1455.00		NIST Webbook
rinpol	1440.00		NIST Webbook
rinpol	1423.00		NIST Webbook
rinpol	1404.00		NIST Webbook
rinpol	1409.00		NIST Webbook
rinpol	1409.00		NIST Webbook
ripol	1791.00		NIST Webbook
ripol	1818.00		NIST Webbook
ripol	1844.00		NIST Webbook
ripol	1800.00		NIST Webbook
ripol	1800.00		NIST Webbook
tb	508.57	K	Joback Method
tc	734.19	K	Joback Method
tf	313.61	K	Joback Method
vc	0.560	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	354.54	J/mol×K	508.57	Joback Method
cpg	374.91	J/mol×K	546.17	Joback Method
cpg	393.60	J/mol×K	583.78	Joback Method
cpg	410.83	J/mol×K	621.38	Joback Method
cpg	426.79	J/mol×K	658.99	Joback Method
cpg	441.72	J/mol×K	696.59	Joback Method
cpg	455.81	J/mol×K	734.19	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=R237708&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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume