Adamantane, 1,3-dichloro

Other names: 1,3-dichloroadamantane
Inchi: InChI=1S/C10H14Cl2/c11-9-2-7-1-8(4-9)5-10(12,3-7)6-9/h7-8H,1-6H2
InchiKey: DZLCQHWJVJXVES-UHFFFAOYSA-N
Formula: C10H14Cl2
SMILES: ClC12CC3CC(C1)CC(Cl)(C3)C2
Mol. weight [g/mol]: 205.12
CAS: 16104-50-0

Physical Properties

Property code	Value	Unit	Source
gf	160.92	kJ/mol	Joback Method
hf	-58.83	kJ/mol	Joback Method
hfus	10.83	kJ/mol	Joback Method
hvap	43.92	kJ/mol	Joback Method
log10ws	-3.74		Crippen Method
logp	3.555		Crippen Method
mcvol	143.660	ml/mol	McGowan Method
pc	3156.17	kPa	Joback Method
rinpol	1453.00		NIST Webbook
rinpol	1453.00		NIST Webbook
rinpol	1453.00		NIST Webbook
ripol	2013.00		NIST Webbook
ripol	2013.00		NIST Webbook
tb	523.36	K	Joback Method
tc	768.67	K	Joback Method
tf	356.16	K	Joback Method
vc	0.551	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	338.92	J/mol×K	523.36	Joback Method
cpg	357.11	J/mol×K	564.24	Joback Method
cpg	373.44	J/mol×K	605.13	Joback Method

cpg	388.29	J/mol×K	646.01	Joback Method
cpg	402.07	J/mol×K	686.90	Joback Method
cpg	415.18	J/mol×K	727.78	Joback Method
cpg	427.99	J/mol×K	768.67	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C16104500&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume