1,3,5-trichloroadamantane

Inchi: InChI=1S/C10H13Cl3/c11-8-1-7-2-9(12,4-8)6-10(13,3-7)5-8/h7H,1-6H2
InchiKey: WJUXAPLLOUYXEF-UHFFFAOYSA-N
Formula: C10H13Cl3
SMILES: ClC12CC3CC(Cl)(C1)CC(Cl)(C3)C2
Mol. weight [g/mol]: 239.57

Physical Properties

Property code	Value	Unit	Source
gf	143.50	kJ/mol	Joback Method
hf	-59.33	kJ/mol	Joback Method
hfus	8.73	kJ/mol	Joback Method
hvap	47.16	kJ/mol	Joback Method
log10ws	-4.25		Crippen Method
logp	3.917		Crippen Method
mcvol	155.900	ml/mol	McGowan Method
pc	3184.73	kPa	Joback Method
rinpol	1582.00		NIST Webbook
rinpol	1582.00		NIST Webbook
rinpol	1582.00		NIST Webbook
tb	561.03	K	Joback Method
tc	821.78	K	Joback Method
tf	409.98	K	Joback Method
vc	0.599	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	366.38	J/mol×K	561.03	Joback Method
cpg	382.39	J/mol×K	604.49	Joback Method
cpg	396.75	J/mol×K	647.95	Joback Method
cpg	410.08	J/mol×K	691.40	Joback Method
cpg	423.01	J/mol×K	734.86	Joback Method
cpg	436.16	J/mol×K	778.32	Joback Method
cpg	450.15	J/mol×K	821.78	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R237684&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