2-Chloroadamantane

Other names: Tricyclo[3.3.1.1(3,7)-]decane, 2-chloro-
Adamantane, 2-chloro
2-chlorotricyclo[3.3.1.13,7]decane
Inchi: InChI=1S/C10H15Cl/c11-10-8-2-6-1-7(4-8)5-9(10)3-6/h6-10H,1-5H2
InchiKey: DPCLLPAHJSYBTE-UHFFFAOYSA-N
Formula: C10H15Cl
SMILES: ClC1C2CC3CC(C2)CC1C3
Mol. weight [g/mol]: 170.68
CAS: 7346-41-0

Physical Properties

Property code	Value	Unit	Source
gf	176.12	kJ/mol	Joback Method
hf	-93.91	kJ/mol	Joback Method
hfus	20.30	kJ/mol	Joback Method
hsub	61.50 ± 0.80	kJ/mol	NIST Webbook
hvap	41.53	kJ/mol	Joback Method
log10ws	-2.99		Crippen Method
logp	3.050		Crippen Method
mcvol	131.420	ml/mol	McGowan Method
pc	2871.95	kPa	Joback Method
rinpol	1342.00		NIST Webbook
rinpol	1342.00		NIST Webbook
rinpol	1404.00		NIST Webbook
rinpol	1376.00		NIST Webbook
rinpol	1350.00		NIST Webbook
rinpol	1361.00		NIST Webbook
rinpol	1342.00		NIST Webbook
rinpol	1350.00		NIST Webbook
rinpol	1345.00		NIST Webbook
ripol	1765.00		NIST Webbook
ripol	1791.00		NIST Webbook
ripol	1738.00		NIST Webbook
ripol	1741.00		NIST Webbook
ripol	1745.00		NIST Webbook
tb	480.78	K	Joback Method
tc	700.35	K	Joback Method

tf	274.20	K	Joback Method
vc	0.505	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	307.29	J/mol×K	480.78	Joback Method
cpg	327.56	J/mol×K	517.38	Joback Method
cpg	346.41	J/mol×K	553.97	Joback Method
cpg	363.92	J/mol×K	590.57	Joback Method
cpg	380.20	J/mol×K	627.16	Joback Method
cpg	395.33	J/mol×K	663.76	Joback Method
cpg	409.42	J/mol×K	700.35	Joback Method
dvisc	0.0008313	Pa×s	274.20	Joback Method
dvisc	0.0009807	Pa×s	308.63	Joback Method
dvisc	0.0011192	Pa×s	343.06	Joback Method
dvisc	0.0012468	Pa×s	377.49	Joback Method
dvisc	0.0013641	Pa×s	411.92	Joback Method
dvisc	0.0014719	Pa×s	446.35	Joback Method
dvisc	0.0015711	Pa×s	480.78	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C7346410&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
dvisc: Dynamic viscosity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions

hsub:	Enthalpy of sublimation 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