1-Bromoadamantane

Other names:	1-adamantyl bromide 1-bromotricyclo[3.3.1.1(3,7)]decane 1-bromotricyclo[3.3.1.13,7]decane Tricyclo[3.3.1.1(3,7)-]decane, 1-bromo- adamantane, 1-bromo- adamantyl bromide tricyclo[3.3.1.1(3,7)]decane, 1-bromo-
Inchi:	InChI=1S/C10H15Br/c11-10-4-7-1-8(5-10)3-9(2-7)6-10/h7-9H,1-6H2
InchiKey:	VQHPRVYDKRESCL-UHFFFAOYSA-N
Formula:	C10H15Br
SMILES:	BrC12CC3CC(CC(C3)C1)C2
Mol. weight [g/mol]:	215.13
CAS:	768-90-1

Physical Properties

Property code	Value	Unit	Source
gf	204.59	kJ/mol	Joback Method
hf	-16.26	kJ/mol	Joback Method
hfus	1.26	kJ/mol	Relationship between the two-component system 1-Br-adamantane + 1-Cl-adamantane and the high-pressure properties of the pure components
hfus	0.00	kJ/mol	Thermodynamic properties of 1-bromoadamantane in the condensed state and molecular disorder in its crystals
hvap	42.74	kJ/mol	Joback Method
ie	9.20	eV	NIST Webbook
ie	9.30 ± 0.06	eV	NIST Webbook
ie	9.40	eV	NIST Webbook
ie	9.63 ± 0.01	eV	NIST Webbook
log10ws	-3.51		Crippen Method
logp	3.350		Crippen Method
mcvol	136.680	ml/mol	McGowan Method
pc	3534.66	kPa	Joback Method
rinpol	1386.00		NIST Webbook
rinpol	1386.00		NIST Webbook

rinpol	1382.00		NIST Webbook
rinpol	1382.00		NIST Webbook
rinpol	1389.00		NIST Webbook
rinpol	1389.00		NIST Webbook
rinpol	1382.00		NIST Webbook
rinpol	1403.00		NIST Webbook
rinpol	1382.00		NIST Webbook
rinpol	1436.00		NIST Webbook
rinpol	1386.00		NIST Webbook
rinpol	1419.00		NIST Webbook
ripol	1837.00		NIST Webbook
ripol	1809.00		NIST Webbook
ripol	1817.00		NIST Webbook
ripol	1817.00		NIST Webbook
tb	514.42	K	Joback Method
tc	755.29	K	Joback Method
tf	396.50 ± 0.20	K	NIST Webbook
vc	0.517	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	377.26	J/mol×K	634.86	Joback Method
cpg	392.15	J/mol×K	675.00	Joback Method
cpg	406.05	J/mol×K	715.15	Joback Method
cpg	324.02	J/mol×K	514.42	Joback Method
cpg	343.46	J/mol×K	554.57	Joback Method
cpg	361.12	J/mol×K	594.71	Joback Method
cpg	419.23	J/mol×K	755.29	Joback Method
hfust	0.88	kJ/mol	279.00	NIST Webbook
hfust	3.83	kJ/mol	396.50	NIST Webbook
hfust	6.93	kJ/mol	310.50	NIST Webbook
hfust	3.97	kJ/mol	360.00	NIST Webbook
hfust	3.83	kJ/mol	396.50	NIST Webbook
hvapt	71.77	kJ/mol	303.00	The thermodynamic properties of 1-bromoadamantane in the gaseous state
sfust	9.66	J/mol×K	396.50	NIST Webbook
sfust	22.32	J/mol×K	310.50	NIST Webbook
sfust	3.15	J/mol×K	279.00	NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Thermodynamic properties of 1-bromoadamantane in the condensed state and molecular disorder in its crystals:	https://www.doi.org/10.1016/j.jct.2004.10.005
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Thermochemistry of 1-bromoadamantane in binary mixtures of water aprotic solvent:	https://www.doi.org/10.1016/j.tca.2005.11.035
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C768901&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Relationship between the two-component system 1-Br-adamantane + 1-Cl-adamantane and the high pressure properties of the pure components:	https://www.doi.org/10.1016/j.fluid.2017.07.020
The thermodynamic properties of 1-bromoadamantane in the gaseous state:	https://www.doi.org/10.1016/j.tca.2005.06.043

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
hfust:	Enthalpy of fusion at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
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
sfust:	Entropy of fusion at a given temperature
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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