1-Bromo-3,5-dimethyladamantane

Other names: 1-Bromo-3,5-dimethyladamantane
3,5-dimethyl-1-bromoadamantane
1-bromo-3,5-dimethyltricyclo[3.3.1.13,7]decane
Inchi: InChI=1S/C12H19Br/c1-10-3-9-4-11(2,6-10)8-12(13,5-9)7-10/h9H,3-8H2,1-2H3
InchiKey: QUCXLVDIVQWYJR-UHFFFAOYSA-N
Formula: C12H19Br
SMILES: CC12CC3CC(C)(C1)CC(Br)(C3)C2
Mol. weight [g/mol]: 243.19

Physical Properties

Property code	Value	Unit	Source
hf	-183.23	kJ/mol	Cheméo Relay (1.0)
hfus	6.60	kJ/mol	Joback Method
hvap	54.99	kJ/mol	Cheméo Relay (1.0)
ie	9.34	eV	Cheméo Relay (1.0)
logp	4.130		Crippen Method
mcvol	164.860	ml/mol	McGowan Method
pc	3142.03	kPa	Joback Method
rinpol	1417.00		NIST Webbook
rinpol	1432.00		NIST Webbook
rinpol	1448.00		NIST Webbook
rinpol	1401.00		NIST Webbook
ripol	1762.00		NIST Webbook
ripol	1762.00		NIST Webbook
ripol	1815.00		NIST Webbook
ripol	1788.00		NIST Webbook
tb	525.80	K	Cheméo Relay (1.0)
tc	760.99	K	Cheméo Relay (1.0)
tf	286.08	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	418.51	J/mol×K	560.66	Joback Method

cpg	438.26	J/mol×K	602.66	Joback Method
cpg	456.22	J/mol×K	644.65	Joback Method
cpg	472.96	J/mol×K	686.65	Joback Method
cpg	489.07	J/mol×K	728.64	Joback Method
cpg	505.13	J/mol×K	770.64	Joback Method
cpg	521.70	J/mol×K	812.64	Joback Method

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C941377&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg: Ideal gas heat capacity
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hvap: Enthalpy of vaporization at standard conditions
ie: Ionization energy
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