Tricyclo[3.3.1.13,7]decane, 2-bromo-

Other names:	2-Adamantyl bromide
	2-bromo-tricyclo[3.3.1.1(3,7)]decane
	2-bromoadamantane
	2-bromotricyclo[3.3.1.13,7]decane
	Adamantane, 2-bromo-
Inchi:	InChI=1S/C10H15Br/c11-10-8-2-6-1-7(4-8)5-9(10)3-6/h6-10H,1-5H2
InchiKey:	RCXJARRRXOPXBC-UHFFFAOYSA-N
Formula:	C10H15Br
SMILES:	BrC1C2CC3CC(C2)CC1C3
Mol. weight [g/mol]:	215.13

Physical Properties

Property code	Value	Unit	Source
hf	-112.46	kJ/mol	Cheméo Relay (1.0)
hfus	4.20	kJ/mol	Six-membered ring aliphatic compounds: A search for regularities in phase transitions
hvap	57.00	kJ/mol	Cheméo Relay (1.0)
ie	9.31 ± 0.05	eV	NIST Webbook
logp	3.206		Crippen Method
mcvol	136.680	ml/mol	McGowan Method
rinpol	1426.00		NIST Webbook
rinpol	1482.00		NIST Webbook
rinpol	1433.00		NIST Webbook
rinpol	1433.00		NIST Webbook
rinpol	1426.00		NIST Webbook
rinpol	1447.00		NIST Webbook
rinpol	1464.00		NIST Webbook
rinpol	1482.00		NIST Webbook
rinpol	1426.00		NIST Webbook
rinpol	1433.00		NIST Webbook
ripol	1861.00		NIST Webbook
ripol	1891.00		NIST Webbook
ripol	1869.00		NIST Webbook
ripol	1869.00		NIST Webbook
tf	515.46	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	324.71	J/mol×K	509.51	Joback Method
cpg	344.72	J/mol×K	547.93	Joback Method
cpg	363.21	J/mol×K	586.35	Joback Method
cpg	380.30	J/mol×K	624.77	Joback Method
cpg	396.12	J/mol×K	663.19	Joback Method
cpg	410.78	J/mol×K	701.61	Joback Method
cpg	424.41	J/mol×K	740.03	Joback Method
dvisc	0.0014069	Pa×s	304.08	Joback Method
dvisc	0.0015509	Pa×s	338.32	Joback Method
dvisc	0.0016792	Pa×s	372.56	Joback Method
dvisc	0.0017940	Pa×s	406.79	Joback Method
dvisc	0.0018971	Pa×s	441.03	Joback Method
dvisc	0.0019900	Pa×s	475.27	Joback Method
dvisc	0.0020741	Pa×s	509.51	Joback Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

Six-membered ring aliphatic compounds: A search for regularities in phase transitions: https://www.doi.org/10.1016/j.tca.2016.06.014

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C7314854&Units=SI

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

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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tf:	Normal melting (fusion) point