Tricyclo[3.3.1.1(3,7)]decane, 2-bromo-

Other names:	Adamantane, 2-bromo-
	2-Adamantyl bromide
	2-Bromoadamantane
	2-bromotricyclo[3.3.1.13,7]decane
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
CAS:	7314-85-4

Physical Properties

Property code	Value	Unit	Source
gf	202.37	kJ/mol	Joback Method
hf	-51.84	kJ/mol	Joback Method
hfus	21.39	kJ/mol	Joback Method
hvap	43.58	kJ/mol	Joback Method
ie	9.31 ± 0.05	eV	NIST Webbook
log10ws	-3.27		Crippen Method
logp	3.206		Crippen Method
mcvol	136.680	ml/mol	McGowan Method
pc	3228.31	kPa	Joback Method
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	1426.00		NIST Webbook
rinpol	1426.00		NIST Webbook
rinpol	1433.00		NIST Webbook
rinpol	1482.00		NIST Webbook
ripol	1869.00		NIST Webbook
ripol	1869.00		NIST Webbook
ripol	1891.00		NIST Webbook
ripol	1869.00		NIST Webbook

ripol	1861.00		NIST Webbook
tb	509.51	K	Joback Method
tc	740.03	K	Joback Method
tf	304.08	K	Joback Method
vc	0.518	m3/kmol	Joback Method

Temperature Dependent Properties

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

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C7314854&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
hvap:	Enthalpy of vaporization at standard conditions
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume