

Cyclopropyl bromide

Other names:	Bromocyclopropane Cyclopropane, bromo-
Inchi:	InChI=1S/C3H5Br/c4-3-1-2-3/h3H,1-2H2
InchiKey:	LKXYJYDRLBPHRS-UHFFFAOYSA-N
Formula:	C3H5Br
SMILES:	BrC1CC1
Mol. weight [g/mol]:	120.98
CAS:	4333-56-6

Physical Properties

Property code	Value	Unit	Source
gf	49.45	kJ/mol	Joback Method
hf	-6.12	kJ/mol	Joback Method
hfus	6.95	kJ/mol	Joback Method
hvap	28.62	kJ/mol	Joback Method
ie	9.53	eV	NIST Webbook
ie	9.93	eV	NIST Webbook
ie	9.60	eV	NIST Webbook
log10ws	-1.52		Crippen Method
logp	1.544		Crippen Method
mcvol	59.770	ml/mol	McGowan Method
pc	5853.95	kPa	Joback Method
tb	342.00	K	NIST Webbook
tc	544.77	K	Joback Method
tf	201.31	K	Joback Method
vc	0.223	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	77.20	J/molxK	340.94	Joback Method
cpg	85.02	J/molxK	374.91	Joback Method
cpg	92.25	J/molxK	408.88	Joback Method
cpg	98.94	J/molxK	442.86	Joback Method

cpg	105.11	J/molxK	476.83	Joback Method
cpg	110.81	J/molxK	510.80	Joback Method
cpg	116.07	J/molxK	544.77	Joback Method
dvisc	0.0009193	Paxs	201.31	Joback Method
dvisc	0.0007631	Paxs	224.58	Joback Method
dvisc	0.0006560	Paxs	247.85	Joback Method
dvisc	0.0005787	Paxs	271.12	Joback Method
dvisc	0.0005207	Paxs	294.40	Joback Method
dvisc	0.0004759	Paxs	317.67	Joback Method
dvisc	0.0004403	Paxs	340.94	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4333566&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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