

Cyclopentane, 1-bromo-2-chloro-, trans-

Other names:	trans-2-Chlorocyclopentyl Bromide 1-Bromo-2-chlorocyclopentane, (E)-
Inchi:	InChI=1S/C5H8BrCl/c6-4-2-1-3-5(4)7/h4-5H,1-3H2/t4-,5-/m0/s1
InchiKey:	KMVDKCXPHPPHOI-WHFBIAKZSA-N
Formula:	C5H8BrCl
SMILES:	C1C1CCCC1Br
Mol. weight [g/mol]:	183.47
CAS:	14376-82-0

Physical Properties

Property code	Value	Unit	Source
gf	22.45	kJ/mol	Joback Method
hf	-95.80	kJ/mol	Joback Method
hfus	13.19	kJ/mol	Joback Method
hvap	37.49	kJ/mol	Joback Method
ie	10.23 ± 0.02	eV	NIST Webbook
log10ws	-2.62		Crippen Method
logp	2.541		Crippen Method
mcvol	100.190	ml/mol	McGowan Method
pc	4333.96	kPa	Joback Method
tb	428.00	K	Joback Method
tc	655.09	K	Joback Method
tf	242.49	K	Joback Method
vc	0.366	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	166.67	J/mol×K	428.00	Joback Method
cpg	178.87	J/mol×K	465.85	Joback Method
cpg	190.30	J/mol×K	503.70	Joback Method
cpg	200.99	J/mol×K	541.54	Joback Method
cpg	210.99	J/mol×K	579.39	Joback Method
cpg	220.31	J/mol×K	617.24	Joback Method

cpg	229.00	J/mol×K	655.09	Joback Method
dvisc	0.0024293	Paxs	242.49	Joback Method
dvisc	0.0015962	Paxs	273.41	Joback Method
dvisc	0.0011422	Paxs	304.33	Joback Method
dvisc	0.0008694	Paxs	335.25	Joback Method
dvisc	0.0006930	Paxs	366.16	Joback Method
dvisc	0.0005722	Paxs	397.08	Joback Method
dvisc	0.0004857	Paxs	428.00	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C14376820&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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