

Cyclopentane, 1-bromo-2-fluoro-, trans-

Other names:	trans-1-Bromo-2-Fluorocyclopentane trans-2-Fluorocyclopentyl Bromide 1-Bromo-2-fluorocyclopentane, (E)-
Inchi:	InChI=1S/C5H8BrF/c6-4-2-1-3-5(4)7/h4-5H,1-3H2/t4-,5-/m0/s1
InchiKey:	GITCXTAKUHIPRH-WHFBIAKZSA-N
Formula:	C5H8BrF
SMILES:	FC1CCCC1Br
Mol. weight [g/mol]:	167.02
CAS:	51422-73-2

Physical Properties

Property code	Value	Unit	Source
gf	-160.43	kJ/mol	Joback Method
hf	-276.17	kJ/mol	Joback Method
hfus	12.08	kJ/mol	Joback Method
hvap	32.29	kJ/mol	Joback Method
ie	10.25 ± 0.02	eV	NIST Webbook
log10ws	-2.32		Crippen Method
logp	2.272		Crippen Method
mcvol	89.720	ml/mol	McGowan Method
pc	4288.66	kPa	Joback Method
tb	389.84	K	Joback Method
tc	596.24	K	Joback Method
tf	213.16	K	Joback Method
vc	0.336	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	149.12	J/molxK	389.84	Joback Method
cpg	161.20	J/molxK	424.24	Joback Method
cpg	172.61	J/molxK	458.64	Joback Method
cpg	183.39	J/molxK	493.04	Joback Method
cpg	193.54	J/molxK	527.44	Joback Method

cpg	203.11	J/mol×K	561.84	Joback Method
cpg	212.10	J/mol×K	596.24	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C51422732&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvac:	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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