Cyclohexane, 1-bromo-2-fluoro-, trans-

Other names: trans-1-Bromo-2-Fluorocyclohexane
trans-2-Fluorocyclohexyl Bromide
Inchi: InChI=1S/C6H10BrF/c7-5-3-1-2-4-6(5)8/h5-6H,1-4H2/t5-,6-/m0/s1
InchiKey: AZQRVGXSORXOCR-WDSKDSINSA-N
Formula: C6H10BrF
SMILES: FC1CCCCC1Br
Mol. weight [g/mol]: 181.05
CAS: 17170-96-6

Physical Properties

Property code	Value	Unit	Source
gf	-164.11	kJ/mol	Joback Method
hf	-302.97	kJ/mol	Joback Method
hfus	12.57	kJ/mol	Joback Method
hvap	34.69	kJ/mol	Joback Method
ie	10.18 ± 0.02	eV	NIST Webbook
ie	10.05	eV	NIST Webbook
log10ws	-2.74		Crippen Method
logp	2.662		Crippen Method
mcvol	103.810	ml/mol	McGowan Method
pc	3916.03	kPa	Joback Method
tb	416.99	K	Joback Method
tc	630.08	K	Joback Method
tf	220.91	K	Joback Method
vc	0.384	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	185.59	J/mol×K	416.99	Joback Method
cpg	199.93	J/mol×K	452.50	Joback Method
cpg	213.50	J/mol×K	488.02	Joback Method
cpg	226.33	J/mol×K	523.53	Joback Method
cpg	238.42	J/mol×K	559.05	Joback Method

cpg	249.81	J/mol×K	594.56	Joback Method
cpg	260.51	J/mol×K	630.08	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C17170966&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
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