1,2-Dibromo-1-chloro-1,2,2-trifluoroethane

Other names:	1,2-DIBROMOCHLOROTRIFLUOROETHANE
	1,2-Dibromo-1-chlorotrifluoroethane
	1,2-Dibromotrifluorochloroethane
	1-Chloro-1,2-dibromo-1,2,2-trifluoro ethane
	2-CHLORO-1,2-DIBROMO-1,1,2-TRIFLUOROETHANE
	Ethane, 1,2-dibromo-1-chloro-1,2,2-trifluoro-
	FREON 113B2
Inchi:	InChI=1S/C2Br2ClF3/c3-1(5,6)2(4,7)8
InchiKey:	OVZATIUQXBLIQT-UHFFFAOYSA-N
Formula:	C2Br2ClF3
SMILES:	FC(F)(Br)C(F)(Cl)Br
Mol. weight [g/mol]:	276.28
CAS:	354-51-8

Physical Properties

Property code	Value	Unit	Source
af	0.2480		KDB
gf	-596.08	kJ/mol	Joback Method
hf	-653.52	kJ/mol	Joback Method
hfus	10.12	kJ/mol	Joback Method
hvap	35.00 ± 0.10	kJ/mol	NIST Webbook
hvap	35.11	kJ/mol	NIST Webbook
log10ws	-3.44		Crippen Method
logp	3.231		Crippen Method
mcvol	91.590	ml/mol	McGowan Method
pc	3610.00	kPa	KDB
tb	366.50 ± 0.50	K	NIST Webbook
tb	366.00	K	NIST Webbook
tb	366.00	K	KDB
tc	560.70	K	NIST Webbook
tc	560.70	K	KDB
tf	182.70	K	KDB
vc	0.368	m3/kmol	KDB
zc	0.2849630		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	162.48	J/mol×K	617.56	Joback Method
cpg	145.28	J/mol×K	441.48	Joback Method
cpg	149.99	J/mol×K	476.69	Joback Method
cpg	154.00	J/mol×K	511.91	Joback Method
cpg	157.38	J/mol×K	547.13	Joback Method
cpg	160.18	J/mol×K	582.35	Joback Method
cpg	139.80	J/mol×K	406.26	Joback Method
hvapt	31.17	kJ/mol	366.00	NIST Webbook
hvapt	31.40	kJ/mol	385.50	NIST Webbook
hvapt	34.20 ± 0.10	kJ/mol	313.00	NIST Webbook
hvapt	33.50 ± 0.10	kJ/mol	328.00	NIST Webbook
hvapt	32.60 ± 0.10	kJ/mol	343.00	NIST Webbook
hvapt	31.60 ± 0.10	kJ/mol	358.00	NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method
KDB: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1533
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C354518&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

af: Acentric Factor
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
hvapt: Enthalpy of vaporization at a given temperature
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
zc:	Critical Compressibility