

Chloro dibromo fluoro methane

Inchi:	InChI=1S/CBr2CIF/c2-1(3,4)5
InchiKey:	HEDKQVNHJZBFQR-UHFFFAOYSA-N
Formula:	CBr2CIF
SMILES:	FC(Cl)(Br)Br
Mol. weight [g/mol]:	226.27
CAS:	353-55-9

Physical Properties

Property code	Value	Unit	Source
gf	-217.72	kJ/mol	Joback Method
hf	-231.91	kJ/mol	Joback Method
hfus	8.78	kJ/mol	Joback Method
hvap	32.96	kJ/mol	Joback Method
log10ws	-2.71		Crippen Method
logp	2.596		Crippen Method
mcvol	73.960	ml/mol	McGowan Method
pc	6514.14	kPa	Joback Method
tb	388.07	K	Joback Method
tc	612.13	K	Joback Method
tf	253.56	K	Joback Method
vc	0.272	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	88.45	J/molxK	388.07	Joback Method
cpg	91.66	J/molxK	425.41	Joback Method
cpg	94.36	J/molxK	462.76	Joback Method
cpg	96.60	J/molxK	500.10	Joback Method
cpg	98.42	J/molxK	537.44	Joback Method
cpg	99.88	J/molxK	574.79	Joback Method
cpg	101.01	J/molxK	612.13	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=C353559&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
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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