Dibromo fluoroacetonitrile

Inchi: InChI=1S/C2Br2FN/c3-2(4,5)1-6
InchiKey: JFEAQFSERNFDSJ-UHFFFAOYSA-N
Formula: C2Br2FN
SMILES: N#CC(F)(Br)Br
Mol. weight [g/mol]: 216.84
CAS: 6698-74-4

Physical Properties

Property code	Value	Unit	Source
gf	-64.19	kJ/mol	Joback Method
hf	-71.93	kJ/mol	Joback Method
hfus	8.68	kJ/mol	Joback Method
hvap	41.28	kJ/mol	Joback Method
log10ws	-2.35		Crippen Method
logp	1.923		Crippen Method
mcvol	77.190	ml/mol	McGowan Method
pc	5713.21	kPa	Joback Method
tb	475.60	K	Joback Method
tc	714.25	K	Joback Method
tf	299.90	K	Joback Method
vc	0.304	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	108.28	J/mol×K	475.60	Joback Method
cpg	111.18	J/mol×K	515.37	Joback Method
cpg	113.62	J/mol×K	555.15	Joback Method
cpg	115.63	J/mol×K	594.92	Joback Method
cpg	117.29	J/mol×K	634.70	Joback Method
cpg	118.64	J/mol×K	674.47	Joback Method
cpg	119.75	J/mol×K	714.25	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6698744&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

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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