1,2-Dibromo-4,5-difluorobenzene

Other names: Benzene, 1,2-dibromo-4,5-difluoro-
Inchi: InChI=1S/C6H2Br2F2/c7-3-1-5(9)6(10)2-4(3)8/h1-2H
InchiKey: JTEZQWOKRHOKDG-UHFFFAOYSA-N
Formula: C6H2Br2F2
SMILES: Fc1cc(Br)c(Br)cc1F
Mol. weight [g/mol]: 271.88
CAS: 64695-78-9

Physical Properties

Property code	Value	Unit	Source
gf	-277.82	kJ/mol	Joback Method
hf	-304.61	kJ/mol	Joback Method
hfus	20.90	kJ/mol	Joback Method
hvap	44.45	kJ/mol	Joback Method
ie	9.13 ± 0.02	eV	NIST Webbook
log10ws	-4.46		Crippen Method
logp	3.490		Crippen Method
mcvol	110.180	ml/mol	McGowan Method
pc	4691.31	kPa	Joback Method
tb	509.16	K	Joback Method
tc	740.99	K	Joback Method
tf	342.14	K	Joback Method
vc	0.423	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	179.02	J/mol×K	509.16	Joback Method
cpg	185.44	J/mol×K	547.80	Joback Method
cpg	191.39	J/mol×K	586.44	Joback Method
cpg	196.90	J/mol×K	625.08	Joback Method
cpg	201.99	J/mol×K	663.71	Joback Method
cpg	206.70	J/mol×K	702.35	Joback Method
cpg	211.05	J/mol×K	740.99	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C64695789&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