2,5-Dibromobenzotrifluoride

Other names:	2,5-Dibromobenzotrifloride
	Benzene, 1,4-dibromo-2-(trifluoromethyl)-
	Toluene, 2,5-dibromo-alpha,alpha,alpha-trifluoro-
	1,4-dibromo-2-(trifluoromethyl)benzene
Inchi:	InChI=1S/C7H3Br2F3/c8-4-1-2-6(9)5(3-4)7(10,11)12/h1-3H
InchiKey:	VWKFJAOCLPPQGR-UHFFFAOYSA-N
Formula:	C7H3Br2F3
SMILES:	FC(F)(F)c1cc(Br)ccc1Br
Mol. weight [g/mol]:	303.90
CAS:	7657-09-2

Physical Properties

Property code	Value	Unit	Source
gf	-451.74	kJ/mol	Joback Method
hf	-518.64	kJ/mol	Joback Method
hfus	19.55	kJ/mol	Joback Method
hvap	43.90	kJ/mol	Joback Method
log10ws	-4.90		Crippen Method
logp	4.230		Crippen Method
mcvol	126.040	ml/mol	McGowan Method
pc	4072.51	kPa	Joback Method
tb	523.10	K	Joback Method
tc	752.20	K	Joback Method
tf	343.90	K	Joback Method
vc	0.486	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	232.23	J/mol×K	523.10	Joback Method
cpg	240.60	J/mol×K	561.28	Joback Method
cpg	248.16	J/mol×K	599.47	Joback Method
cpg	255.00	J/mol×K	637.65	Joback Method
cpg	261.18	J/mol×K	675.84	Joback Method

cpg	266.77	J/mol×K	714.02	Joback Method
cpg	271.83	J/mol×K	752.20	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7657092&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