4-Amino-3,5-dibromobenzotrifluoride

Inchi: InChI=1S/C7H4Br2F3N/c8-4-1-3(7(10,11)12)2-5(9)6(4)13/h1-2H,13H2
InchiKey: DRSMEHXBOXHXDX-UHFFFAOYSA-N
Formula: C7H4Br2F3N
SMILES: Nc1c(Br)cc(C(F)(F)F)cc1Br
Mol. weight [g/mol]: 318.92
CAS: 72678-19-4

Physical Properties

Property code	Value	Unit	Source
gf	-394.92	kJ/mol	Joback Method
hf	-496.32	kJ/mol	Joback Method
hfus	24.35	kJ/mol	Joback Method
hvap	55.20	kJ/mol	Joback Method
log10ws	-4.53		Crippen Method
logp	3.813		Crippen Method
mcvol	136.020	ml/mol	McGowan Method
pc	4299.92	kPa	Joback Method
tb	600.61	K	Joback Method
tc	839.21	K	Joback Method
tf	439.68	K	Joback Method
vc	0.515	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	276.13	J/mol×K	600.61	Joback Method
cpg	283.84	J/mol×K	640.38	Joback Method
cpg	290.82	J/mol×K	680.14	Joback Method
cpg	297.17	J/mol×K	719.91	Joback Method
cpg	302.93	J/mol×K	759.68	Joback Method
cpg	308.19	J/mol×K	799.45	Joback Method
cpg	313.02	J/mol×K	839.21	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C72678194&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
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