4-Amino-3-bromobenzotrifluoride

Other names: 2-bromo-4-trifluoromethylaniline
Inchi: InChI=1S/C7H5BrF3N/c8-5-3-4(7(9,10)11)1-2-6(5)12/h1-3H,12H2
InchiKey: QKRJIXSZTKOFTD-UHFFFAOYSA-N
Formula: C7H5BrF3N
SMILES: Nc1ccc(C(F)(F)F)cc1Br
Mol. weight [g/mol]: 240.02

Physical Properties

Property code	Value	Unit	Source
hfus	19.46	kJ/mol	Joback Method
ie	8.61	eV	Cheméo Relay (1.0)
log10ws	-3.04		Cheméo Relay (1.0)
logp	3.050		Crippen Method
mcvol	118.520	ml/mol	McGowan Method
tb	495.58	K	Cheméo Relay (1.0)
tf	338.78	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	248.96	J/mol×K	529.47	Joback Method
cpg	258.25	J/mol×K	566.76	Joback Method
cpg	266.76	J/mol×K	604.04	Joback Method
cpg	274.55	J/mol×K	641.33	Joback Method
cpg	281.67	J/mol×K	678.62	Joback Method
cpg	288.17	J/mol×K	715.91	Joback Method
cpg	294.12	J/mol×K	753.19	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C57946631&Units=SI

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point