2-Bromo-4,6-difluoroaniline

Other names: Benzenamine, 2-bromo-4,6-difluoro-
Inchi: InChI=1S/C6H4BrF2N/c7-4-1-3(8)2-5(9)6(4)10/h1-2H,10H2
InchiKey: WUJKFVGKLTWVSQ-UHFFFAOYSA-N
Formula: C6H4BrF2N
SMILES: Nc1c(F)cc(F)cc1Br
Mol. weight [g/mol]: 208.00
CAS: 444-14-4

Physical Properties

Property code	Value	Unit	Source
gf	-225.69	kJ/mol	Joback Method
hf	-297.15	kJ/mol	Joback Method
hfus	20.81	kJ/mol	Joback Method
hvap	48.65	kJ/mol	Joback Method
log10ws	-2.93		Crippen Method
logp	2.310		Crippen Method
mcvol	102.660	ml/mol	McGowan Method
pc	4615.13	kPa	Joback Method
tb	515.53	K	Joback Method
tc	741.84	K	Joback Method
tf	365.60	K	Joback Method
vc	0.391	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	194.91	J/mol×K	515.53	Joback Method
cpg	202.38	J/mol×K	553.25	Joback Method
cpg	209.38	J/mol×K	590.97	Joback Method
cpg	215.92	J/mol×K	628.68	Joback Method
cpg	222.02	J/mol×K	666.40	Joback Method
cpg	227.71	J/mol×K	704.12	Joback Method
cpg	233.00	J/mol×K	741.84	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C444144&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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