4-Bromo-2,5-difluoronitrobenzene

Inchi: InChI=1S/C6H2BrF2NO2/c7-3-1-5(9)6(10(11)12)2-4(3)8/h1-2H
InchiKey: GJFYMYJYPARISZ-UHFFFAOYSA-N
Formula: C6H2BrF2NO2
SMILES: O=[N+]([O-])c1cc(F)c(Br)cc1F
Mol. weight [g/mol]: 237.99
CAS: 167415-27-2

Physical Properties

Property code	Value	Unit	Source
gf	-256.59	kJ/mol	Joback Method
hf	-341.70	kJ/mol	Joback Method
hfus	26.98	kJ/mol	Joback Method
hvap	54.60	kJ/mol	Joback Method
log10ws	-3.95		Crippen Method
logp	2.635		Crippen Method
mcvol	110.100	ml/mol	McGowan Method
pc	4345.39	kPa	Joback Method
tb	594.84	K	Joback Method
tc	840.05	K	Joback Method
tf	425.95	K	Joback Method
vc	0.444	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	220.82	J/mol×K	594.84	Joback Method
cpg	228.02	J/mol×K	635.71	Joback Method
cpg	234.64	J/mol×K	676.58	Joback Method
cpg	240.73	J/mol×K	717.44	Joback Method
cpg	246.32	J/mol×K	758.31	Joback Method
cpg	251.42	J/mol×K	799.18	Joback Method
cpg	256.09	J/mol×K	840.05	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C167415272&Units=SI

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