1-Bromo-3,4-difluorobenzene

Other names:	4-Bromo-1,2-difluorobenzene
	Benzene, 4-bromo-1,2-difluoro-
Inchi:	InChI=1S/C6H3BrF2/c7-4-1-2-5(8)6(9)3-4/h1-3H
InchiKey:	YMQPKONILWWJQG-UHFFFAOYSA-N
Formula:	C6H3BrF2
SMILES:	Fc1ccc(Br)cc1F
Mol. weight [g/mol]:	192.99
CAS:	348-61-8

Physical Properties

Property code	Value	Unit	Source
gf	-282.51	kJ/mol	Joback Method
hf	-319.47	kJ/mol	Joback Method
hfus	16.00	kJ/mol	Joback Method
hvap	37.35	kJ/mol	Joback Method
log10ws	-3.30		Crippen Method
logp	2.727		Crippen Method
mcvol	92.680	ml/mol	McGowan Method
pc	4362.63	kPa	Joback Method
tb	438.02	K	Joback Method
tc	651.05	K	Joback Method
tf	269.82	K	Joback Method
vc	0.361	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	152.73	J/mol×K	438.02	Joback Method
cpg	160.24	J/mol×K	473.53	Joback Method
cpg	167.26	J/mol×K	509.03	Joback Method
cpg	173.84	J/mol×K	544.54	Joback Method
cpg	179.98	J/mol×K	580.04	Joback Method
cpg	185.71	J/mol×K	615.55	Joback Method
cpg	191.05	J/mol×K	651.05	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=C348618&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