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

Physical Properties

Property code	Value	Unit	Source
af	0.3335		Cheméo Relay (1.0)
hf	-238.64	kJ/mol	Cheméo Relay (1.0)
hfus	16.00	kJ/mol	Joback Method
hvap	47.05	kJ/mol	Cheméo Relay (1.0)
ie	9.19 ± 0.02	eV	NIST Webbook
log10ws	-3.02		Cheméo Relay (1.0)
logp	2.727		Crippen Method
mcvol	92.680	ml/mol	McGowan Method
pc	4362.63	kPa	Joback Method
tb	423.70	K	NIST Webbook
tb	423.50 ± 0.50	K	NIST Webbook
tc	634.20	K	Cheméo Relay (1.0)
tf	254.28	K	Cheméo Relay (1.0)

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

Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C348618&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

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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