1-BROMO-3,5-DIFLUOROBENZENE

Other names: Benzene, 1-bromo-3,5-difluoro-
Inchi: InChI=1S/C6H3BrF2/c7-4-1-5(8)3-6(9)2-4/h1-3H
InchiKey: JHLKSIOJYMGSMB-UHFFFAOYSA-N
Formula: C6H3BrF2
SMILES: Fc1cc(F)cc(Br)c1
Mol. weight [g/mol]: 192.99

Physical Properties

Property code	Value	Unit	Source
hfus	16.00	kJ/mol	Joback Method
hvap	45.31	kJ/mol	Cheméo Relay (1.0)
ie	9.39	eV	Cheméo Relay (1.0)
log10ws	-3.26		Cheméo Relay (1.0)
logp	2.727		Crippen Method
mcvol	92.680	ml/mol	McGowan Method
tb	413.20	K	NIST Webbook
tb	413.00	K	NIST Webbook
tf	260.36	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=C461961&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

cpg:	Ideal gas heat capacity
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
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point