2-Bromo-5-fluorotoluene

Other names: 3-Fluoro-6-bromotoluene
Benzene, 1-bromo-4-fluoro-2-methyl-
Inchi: InChI=1S/C7H6BrF/c1-5-4-6(9)2-3-7(5)8/h2-4H,1H3
InchiKey: RJPNVPITBYXBNB-UHFFFAOYSA-N
Formula: C7H6BrF
SMILES: Cc1cc(F)ccc1Br
Mol. weight [g/mol]: 189.03
CAS: 452-63-1

Physical Properties

Property code	Value	Unit	Source
gf	-79.28	kJ/mol	Joback Method
hf	-144.00	kJ/mol	Joback Method
hfus	15.51	kJ/mol	Joback Method
hvap	40.39	kJ/mol	Joback Method
log10ws	-3.44		Crippen Method
logp	2.897		Crippen Method
mcvol	105.000	ml/mol	McGowan Method
pc	4082.92	kPa	Joback Method
tb	461.63	K	Joback Method
tc	683.84	K	Joback Method
tf	280.50	K	Joback Method
vc	0.400	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	181.72	J/mol×K	461.63	Joback Method
cpg	191.09	J/mol×K	498.67	Joback Method
cpg	199.89	J/mol×K	535.70	Joback Method
cpg	208.13	J/mol×K	572.74	Joback Method
cpg	215.85	J/mol×K	609.77	Joback Method
cpg	223.07	J/mol×K	646.81	Joback Method
cpg	229.81	J/mol×K	683.84	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C452631&Units=SI
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

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