3-Bromo-4-hydroxy-5-methoxyphenylacetonitrile

Inchi: InChI=1S/C9H8BrNO2/c1-13-8-5-6(2-3-11)4-7(10)9(8)12/h4-5,12H,2H2,1H3
InchiKey: VMARCRAWRNPBBQ-UHFFFAOYSA-N
Formula: C9H8BrNO2
SMILES: COc1cc(CC#N)cc(Br)c1O
Mol. weight [g/mol]: 242.07
CAS: 81038-44-0

Physical Properties

Property code	Value	Unit	Source
gf	5.93	kJ/mol	Joback Method
hf	-133.82	kJ/mol	Joback Method
hfus	26.09	kJ/mol	Joback Method
hvap	71.56	kJ/mol	Joback Method
log10ws	-2.97		Crippen Method
logp	2.229		Crippen Method
mcvol	144.530	ml/mol	McGowan Method
pc	3881.95	kPa	Joback Method
tb	713.24	K	Joback Method
tc	960.32	K	Joback Method
tf	501.39	K	Joback Method
vc	0.503	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	333.85	J/mol×K	713.24	Joback Method
cpg	342.39	J/mol×K	754.42	Joback Method
cpg	350.42	J/mol×K	795.60	Joback Method
cpg	358.03	J/mol×K	836.78	Joback Method
cpg	365.30	J/mol×K	877.96	Joback Method
cpg	372.29	J/mol×K	919.14	Joback Method
cpg	379.08	J/mol×K	960.32	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C81038440&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

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