2-Bromo-4,5-dimethoxyphenylacetonitrile

Inchi: InChI=1S/C10H10BrNO2/c1-13-9-5-7(3-4-12)8(11)6-10(9)14-2/h5-6H,3H2,1-2H3
InchiKey: OYPMCZMEPRFUFJ-UHFFFAOYSA-N
Formula: C10H10BrNO2
SMILES: COc1cc(Br)c(CC#N)cc1OC
Mol. weight [g/mol]: 256.10
CAS: 51655-39-1

Physical Properties

Property code	Value	Unit	Source
gf	54.34	kJ/mol	Joback Method
hf	-120.84	kJ/mol	Joback Method
hfus	23.70	kJ/mol	Joback Method
hvap	63.85	kJ/mol	Joback Method
log10ws	-3.54		Crippen Method
logp	2.532		Crippen Method
mcvol	158.620	ml/mol	McGowan Method
pc	2823.32	kPa	Joback Method
tb	682.90	K	Joback Method
tc	914.90	K	Joback Method
tf	435.69	K	Joback Method
vc	0.612	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	363.77	J/mol×K	682.90	Joback Method
cpg	374.28	J/mol×K	721.57	Joback Method
cpg	384.13	J/mol×K	760.23	Joback Method
cpg	393.33	J/mol×K	798.90	Joback Method
cpg	401.85	J/mol×K	837.57	Joback Method
cpg	409.69	J/mol×K	876.23	Joback Method
cpg	416.85	J/mol×K	914.90	Joback Method

Sources

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=C51655391&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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