4-Methoxy-5-bromo-dimethylaminobenzene

Inchi: InChI=1S/C9H12BrNO/c1-11(2)7-4-5-9(12-3)8(10)6-7/h4-6H,1-3H3
InchiKey: ZPTYNMDNRYYQSI-UHFFFAOYSA-N
Formula: C9H12BrNO
SMILES: COc1ccc(N(C)C)cc1Br
Mol. weight [g/mol]: 230.10

Physical Properties

Property code	Value	Unit	Source
gf	138.15	kJ/mol	Joback Method
hf	-53.86	kJ/mol	Joback Method
hfus	21.82	kJ/mol	Joback Method
hvap	50.12	kJ/mol	Joback Method
log10ws	-2.66		Crippen Method
logp	2.524		Crippen Method
mcvol	147.260	ml/mol	McGowan Method
pc	3337.38	kPa	Joback Method
rinpol	1633.00		NIST Webbook
rinpol	1633.00		NIST Webbook
tb	542.98	K	Joback Method
tc	763.98	K	Joback Method
tf	357.15	K	Joback Method
vc	0.529	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	310.60	J/mol×K	542.98	Joback Method
cpg	323.64	J/mol×K	579.81	Joback Method
cpg	335.91	J/mol×K	616.65	Joback Method
cpg	347.44	J/mol×K	653.48	Joback Method
cpg	358.26	J/mol×K	690.31	Joback Method
cpg	368.39	J/mol×K	727.15	Joback Method
cpg	377.86	J/mol×K	763.98	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U374811&Units=SI

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume