4-Bromo-alpha-(dimethylamino)-o-cresol

Inchi: InChI=1S/C9H12BrNO/c1-11(2)6-7-5-8(10)3-4-9(7)12/h3-5,12H,6H2,1-2H3
InchiKey: VKWZAKOXYMCAER-UHFFFAOYSA-N
Formula: C9H12BrNO
SMILES: CN(C)Cc1cc(Br)ccc1O
Mol. weight [g/mol]: 230.10
CAS: 42313-79-1

Physical Properties

Property code	Value	Unit	Source
gf	98.16	kJ/mol	Joback Method
hf	-87.48	kJ/mol	Joback Method
hfus	26.81	kJ/mol	Joback Method
hvap	60.06	kJ/mol	Joback Method
log10ws	-2.47		Crippen Method
logp	2.216		Crippen Method
mcvol	147.260	ml/mol	McGowan Method
pc	4162.33	kPa	Joback Method
tb	596.20	K	Joback Method
tc	829.90	K	Joback Method
tf	434.12	K	Joback Method
vc	0.477	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	336.47	J/mol×K	596.20	Joback Method
cpg	348.47	J/mol×K	635.15	Joback Method
cpg	359.57	J/mol×K	674.10	Joback Method
cpg	369.87	J/mol×K	713.05	Joback Method
cpg	379.49	J/mol×K	752.00	Joback Method
cpg	388.52	J/mol×K	790.95	Joback Method
cpg	397.09	J/mol×K	829.90	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=C42313791&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume