4-Chloro-a-(dimethylamino)-o-cresol

Inchi: InChI=1S/C9H12ClNO/c1-11(2)6-7-5-8(10)3-4-9(7)12/h3-5,12H,6H2,1-2H3
InchiKey: WPEGHIRPYPPYDO-UHFFFAOYSA-N
Formula: C9H12ClNO
SMILES: CN(C)Cc1cc(Cl)ccc1O
Mol. weight [g/mol]: 185.65
CAS: 54828-00-1

Physical Properties

Property code	Value	Unit	Source
gf	71.91	kJ/mol	Joback Method
hf	-129.55	kJ/mol	Joback Method
hfus	25.72	kJ/mol	Joback Method
hvap	58.01	kJ/mol	Joback Method
log10ws	-1.99		Crippen Method
logp	2.107		Crippen Method
mcvol	142.000	ml/mol	McGowan Method
pc	3646.53	kPa	Joback Method
tb	567.47	K	Joback Method
tc	791.85	K	Joback Method
tf	404.24	K	Joback Method
vc	0.465	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	325.70	J/mol×K	567.47	Joback Method
cpg	338.04	J/mol×K	604.87	Joback Method
cpg	349.48	J/mol×K	642.26	Joback Method
cpg	360.12	J/mol×K	679.66	Joback Method
cpg	370.04	J/mol×K	717.06	Joback Method
cpg	379.33	J/mol×K	754.46	Joback Method
cpg	388.08	J/mol×K	791.85	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C54828001&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