Clotermine

Inchi: InChI=1S/C10H14ClN/c1-10(2,12)7-8-5-3-4-6-9(8)11/h3-6H,7,12H2,1-2H3
InchiKey: HXCXASJHZQXCKK-UHFFFAOYSA-N
Formula: C10H14ClN
SMILES: CC(C)(N)Cc1ccccc1Cl
Mol. weight [g/mol]: 183.68

Physical Properties

Property code	Value	Unit	Source
gf	193.46	kJ/mol	Joback Method
hf	-15.37	kJ/mol	Joback Method
hfus	17.29	kJ/mol	Joback Method
hvap	54.52	kJ/mol	Joback Method
log10ws	-3.34		Crippen Method
logp	2.620		Crippen Method
mcvol	150.220	ml/mol	McGowan Method
pc	3009.03	kPa	Joback Method
rinpol	1305.00		NIST Webbook
tb	566.59	K	Joback Method
tc	802.25	K	Joback Method
tf	357.00	K	Joback Method
vc	0.554	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	346.63	J/mol×K	566.59	Joback Method
cpg	361.26	J/mol×K	605.87	Joback Method
cpg	374.79	J/mol×K	645.14	Joback Method
cpg	387.29	J/mol×K	684.42	Joback Method
cpg	398.84	J/mol×K	723.70	Joback Method
cpg	409.51	J/mol×K	762.97	Joback Method
cpg	419.38	J/mol×K	802.25	Joback Method

Sources

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=R596428&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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