3-Cl-C6H4CON(CH3)2

Inchi: InChI=1S/C9H10ClNO/c1-11(2)9(12)7-4-3-5-8(10)6-7/h3-6H,1-2H3
InchiKey: JSXDHOISXRKLGG-UHFFFAOYSA-N
Formula: C9H10ClNO
SMILES: CN(C)C(=O)c1cccc(Cl)c1
Mol. weight [g/mol]: 183.63
CAS: 24167-52-0

Physical Properties

Property code	Value	Unit	Source
affp	927.90	kJ/mol	NIST Webbook
basg	896.90	kJ/mol	NIST Webbook
gf	97.61	kJ/mol	Joback Method
hf	-64.82	kJ/mol	Joback Method
hfus	21.54	kJ/mol	Joback Method
hvap	51.74	kJ/mol	Joback Method
log10ws	-2.30		Crippen Method
logp	2.042		Crippen Method
mcvol	137.700	ml/mol	McGowan Method
pc	3295.37	kPa	Joback Method
tb	540.72	K	Joback Method
tc	762.06	K	Joback Method
tf	342.45	K	Joback Method
vc	0.504	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	291.78	J/mol×K	540.72	Joback Method
cpg	304.33	J/mol×K	577.61	Joback Method
cpg	316.02	J/mol×K	614.50	Joback Method
cpg	326.91	J/mol×K	651.39	Joback Method
cpg	337.03	J/mol×K	688.28	Joback Method
cpg	346.41	J/mol×K	725.17	Joback Method
cpg	355.11	J/mol×K	762.06	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=C24167520&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

affp:	Proton affinity
basg:	Gas basicity
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