

Cloponone

Inchi:	InChI=1S/C11H9Cl4NO2/c12-5-8(16-11(18)10(14)15)9(17)6-1-3-7(13)4-2-6/h1-4,8,10H,5
InchiKey:	MLVKMSCFQIQULM-UHFFFAOYSA-N
Formula:	C11H9Cl4NO2
SMILES:	O=C(NC(CCl)C(=O)c1ccc(Cl)cc1)C(Cl)Cl
Mol. weight [g/mol]:	329.01
CAS:	15301-50-5

Physical Properties

Property code	Value	Unit	Source
gf	-76.53	kJ/mol	Joback Method
hf	-290.52	kJ/mol	Joback Method
hfus	35.94	kJ/mol	Joback Method
hvap	79.71	kJ/mol	Joback Method
log10ws	-4.22		Crippen Method
logp	3.050		Crippen Method
mvol	204.170	ml/mol	McGowan Method
pc	2627.15	kPa	Joback Method
rinpol	2011.00		NIST Webbook
tb	789.49	K	Joback Method
tc	1028.56	K	Joback Method
tf	494.87	K	Joback Method
vc	0.774	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	475.53	J/molxK	789.49	Joback Method
cpg	484.59	J/molxK	829.34	Joback Method
cpg	492.79	J/molxK	869.18	Joback Method
cpg	500.18	J/molxK	909.03	Joback Method
cpg	506.83	J/molxK	948.87	Joback Method
cpg	512.78	J/molxK	988.72	Joback Method
cpg	518.10	J/molxK	1028.56	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C15301505&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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