

M-chlorocarbanilic acid, ethyl lactate ester

Inchi:	InChI=1S/C12H14ClNO4/c1-3-17-11(15)8(2)18-12(16)14-10-6-4-5-9(13)7-10/h4-8H,3H2
InchiKey:	ZXUAHEYZOUGLVLU-UHFFFAOYSA-N
Formula:	C12H14ClNO4
SMILES:	CCOC(=O)C(C)OC(=O)Nc1cccc(Cl)c1
Mol. weight [g/mol]:	271.70
CAS:	1149-42-4

Physical Properties

Property code	Value	Unit	Source
gf	-239.88	kJ/mol	Joback Method
hf	-523.10	kJ/mol	Joback Method
hfus	31.84	kJ/mol	Joback Method
hvap	73.99	kJ/mol	Joback Method
log10ws	-3.07		Crippen Method
logp	2.840		Crippen Method
mcvol	193.280	ml/mol	McGowan Method
pc	2555.92	kPa	Joback Method
tb	745.36	K	Joback Method
tc	963.57	K	Joback Method
tf	475.84	K	Joback Method
vc	0.726	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	512.02	J/molxK	745.36	Joback Method
cpg	524.13	J/molxK	781.73	Joback Method
cpg	535.32	J/molxK	818.10	Joback Method
cpg	545.59	J/molxK	854.46	Joback Method
cpg	554.94	J/molxK	890.83	Joback Method
cpg	563.39	J/molxK	927.20	Joback Method
cpg	570.93	J/molxK	963.57	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1149424&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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

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