

(2-Chloro-6-methylphenoxy)acetic acid

Other names:	6-chloro-o-tolyloxyacetic acid
Inchi:	InChI=1S/C9H9ClO3/c1-6-3-2-4-7(10)9(6)13-5-8(11)12/h2-4H,5H2,1H3,(H,11,12)
InchiKey:	WHLKFTSLSDHFMU-UHFFFAOYSA-N
Formula:	C9H9ClO3
SMILES:	<chem>Cc1cccc(Cl)c1OCC(=O)O</chem>
Mol. weight [g/mol]:	200.62
CAS:	19094-75-8

Physical Properties

Property code	Value	Unit	Source
gf	-264.62	kJ/mol	Joback Method
hf	-428.27	kJ/mol	Joback Method
hfus	23.40	kJ/mol	Joback Method
hvap	69.45	kJ/mol	Joback Method
log10ws	-2.27		Crippen Method
logp	2.112		Crippen Method
mcvol	139.460	ml/mol	McGowan Method
pc	3543.08	kPa	Joback Method
tb	647.86	K	Joback Method
tc	854.75	K	Joback Method
tf	405.55	K	Joback Method
vc	0.523	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	323.99	J/molxK	647.86	Joback Method
cpg	364.79	J/molxK	820.27	Joback Method
cpg	357.70	J/molxK	785.79	Joback Method
cpg	350.07	J/molxK	751.31	Joback Method
cpg	341.92	J/molxK	716.82	Joback Method
cpg	333.23	J/molxK	682.34	Joback Method
cpg	371.37	J/molxK	854.75	Joback Method
dvisc	0.0000659	Paxs	647.86	Joback Method

dvisc	0.0000929	Paxs	607.48	Joback Method
dvisc	0.0001375	Paxs	567.09	Joback Method
dvisc	0.0002162	Paxs	526.71	Joback Method
dvisc	0.0003666	Paxs	486.32	Joback Method
dvisc	0.0006838	Paxs	445.94	Joback Method
dvisc	0.0014442	Paxs	405.55	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=C19094758&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
dvisc:	Dynamic viscosity
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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