Meclofenoxate

Other names:	Acetic acid, (4-chlorophenoxy)-, 2-(dimethylamino)ethyl ester (p-Chlorophenoxy)acetic acid «beta»-(dimethylamino)ethyl ester (p-Chlorophenoxy)acetic acid 2-(dimethylamino)ethyl ester 2-(Dimethylamino)ethyl p-chlorophenoxyacetate 2-(Dimethylamino)ethyl-4-(chlorophenoxy)acetate Acephene Acetic acid, (p-chlorophenoxy)-, 2-(dimethylamino)ethyl ester Analux ANP 235 Cerebon Cetrexin Clofenoxin Clophenoxate Deanol p-chlorophenoxyacetate Deanolestere EN 1627 Licidril Meclofenoxane Meclophenoxate Mucidril Proseryl 2-(Dimethylamino)ethyl (p-chlorphenoxy)acetate Centrexin Clopenoxin Acephen Clocete NSC 169411
Inchi:	InChI=1S/C12H16ClNO3/c1-14(2)7-8-16-12(15)9-17-11-5-3-10(13)4-6-11/h3-6H,7-9H2,1
InchiKey:	XZTYGFHCIAKPGJ-UHFFFAOYSA-N
Formula:	C12H16ClNO3
SMILES:	CN(C)CCOC(=O)COc1ccc(Cl)cc1
Mol. weight [g/mol]:	257.71
CAS:	51-68-3

Physical Properties

Property code	Value	Unit	Source

gf	-87.13	kJ/mol	Joback Method
hf	-391.18	kJ/mol	Joback Method
hfus	31.68	kJ/mol	Joback Method
hvap	63.24	kJ/mol	Joback Method
log10ws	-1.80		Crippen Method
logp	1.824		Crippen Method
mcvol	191.710	ml/mol	McGowan Method
pc	2347.36	kPa	Joback Method
rinpol	1790.00		NIST Webbook
rinpol	1770.00		NIST Webbook
rinpol	1790.00		NIST Webbook
tb	654.20	K	Joback Method
tc	860.18	K	Joback Method
tf	420.72	K	Joback Method
vc	0.709	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	484.21	J/mol×K	654.20	Joback Method
cpg	498.32	J/mol×K	688.53	Joback Method
cpg	511.57	J/mol×K	722.86	Joback Method
cpg	523.99	J/mol×K	757.19	Joback Method
cpg	535.59	J/mol×K	791.52	Joback Method
cpg	546.38	J/mol×K	825.85	Joback Method
cpg	556.37	J/mol×K	860.18	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C51683&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Joback Method: https://en.wikipedia.org/wiki/Joback_method

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