Fenoxanil

Other names: Propanamide, N-(1-cyano-1,2-dimethylpropyl)-2-(2,4-dichlorophenoxy)-
Inchi: InChI=1S/C15H18Cl2N2O2/c1-9(2)15(4,8-18)19-14(20)10(3)21-13-6-5-11(16)7-12(13)17
InchiKey: IUOKJNROJISWRO-UHFFFAOYSA-N
Formula: C15H18Cl2N2O2
SMILES: CC(Oc1ccc(Cl)cc1Cl)C(=O)NC(C)(C#N)C(C)C
Mol. weight [g/mol]: 329.22
CAS: 115852-48-7

Physical Properties

Property code	Value	Unit	Source
gf	131.32	kJ/mol	Joback Method
hf	-216.58	kJ/mol	Joback Method
hfus	31.20	kJ/mol	Joback Method
hvap	85.35	kJ/mol	Joback Method
log10ws	-5.12		Crippen Method
logp	3.815		Crippen Method
mcvol	241.730	ml/mol	McGowan Method
pc	1792.42	kPa	Joback Method
rinpol	2269.00		NIST Webbook
rinpol	2240.00		NIST Webbook
rinpol	2270.80		NIST Webbook
rinpol	2269.00		NIST Webbook
tb	878.53	K	Joback Method
tc	1112.28	K	Joback Method
tf	532.34	K	Joback Method
vc	0.927	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	676.64	J/mol×K	878.53	Joback Method
cpg	687.89	J/mol×K	917.49	Joback Method
cpg	698.16	J/mol×K	956.45	Joback Method
cpg	707.51	J/mol×K	995.41	Joback Method

cpg	716.01	J/mol×K	1034.36	Joback Method
cpg	723.72	J/mol×K	1073.32	Joback Method
cpg	730.69	J/mol×K	1112.28	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C115852487&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
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume