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]: 329.23

Physical Properties

Property code	Value	Unit	Source
hfus	31.20	kJ/mol	Joback Method
log10ws	-4.64		Cheméo Relay (1.0)
logp	3.815		Crippen Method
mcvol	241.730	ml/mol	McGowan Method
rinpol	2269.00		NIST Webbook
rinpol	2270.80		NIST Webbook
rinpol	2240.00		NIST Webbook
rinpol	2269.00		NIST Webbook
tf	397.09	K	Cheméo Relay (1.0)

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

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C115852487&Units=SI
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
hfus:	Enthalpy of fusion at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tf:	Normal melting (fusion) point