

Diclofop

Other names: Propanoic acid, 2-[4-(2,4-dichlorophenoxy)phenoxy]-

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Inchi: InChI=1S/C15H12Cl2O4/c1-9(15(18)19)20-11-3-5-12(6-4-11)21-14-7-2-10(16)8-13(14)1

InchiKey: OOLBCHYXZDXLDS-UHFFFAOYSA-N

Formula: C15H12Cl2O4

SMILES: CC(Oc1ccc(Oc2ccc(Cl)cc2Cl)cc1)C(=O)O

Mol. weight [g/mol]: 327.16

CAS: 40843-25-2

Physical Properties

Property code	Value	Unit	Source
gf	-230.69	kJ/mol	Joback Method
hf	-480.29	kJ/mol	Joback Method
hfus	34.45	kJ/mol	Joback Method
hvap	92.15	kJ/mol	Joback Method
log10ws	-4.64		Crippen Method
logp	4.638		Crippen Method
mcvol	218.350	ml/mol	McGowan Method
pc	2535.37	kPa	Joback Method
tb	876.21	K	Joback Method
tc	1105.84	K	Joback Method
tf	549.26	K	Joback Method
vc	0.812	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	582.08	J/molxK	876.21	Joback Method
cpg	591.46	J/molxK	914.48	Joback Method
cpg	599.82	J/molxK	952.75	Joback Method
cpg	607.20	J/molxK	991.03	Joback Method
cpg	613.61	J/molxK	1029.30	Joback Method
cpg	619.06	J/molxK	1067.57	Joback Method
cpg	623.57	J/molxK	1105.84	Joback Method

dvisc	0.0002226	Paxs	549.26	Joback Method
dvisc	0.0001112	Paxs	603.75	Joback Method
dvisc	0.0000623	Paxs	658.24	Joback Method
dvisc	0.0000381	Paxs	712.74	Joback Method
dvisc	0.0000250	Paxs	767.23	Joback Method
dvisc	0.0000174	Paxs	821.72	Joback Method
dvisc	0.0000126	Paxs	876.21	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C40843252&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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