Carbamic acid, (2-(4-phenoxyphenoxy)ethyl)-, ethyl ester

Other names: (2-(4-Phenoxyphenoxy)ethyl)carbamic acid ethyl ester
Ethyl (2-(4-phenoxyphenoxy)ethyl)carbamate
Fenoxycarb
Insegar
Ro 13-5223
ethyl 2-(p-phenoxyphenoxy)ethylcarbamate
ethyl [2-(4-phenoxyphenoxy)ethyl]carbamate

Inchi: InChI=1S/C17H19NO4/c1-2-20-17(19)18-12-13-21-14-8-10-16(11-9-14)22-15-6-4-3-5-7-

InchiKey: HJUFTIJOISQSKQ-UHFFFAOYSA-N

Formula: C17H19NO4

SMILES: CCOC(=O)NCCOc1ccc(Oc2ccccc2)cc1

Mol. weight [g/mol]: 301.34

CAS: 79127-80-3

Physical Properties

Property code	Value	Unit	Source
gf	-47.08	kJ/mol	Joback Method
hf	-388.39	kJ/mol	Joback Method
hfus	37.74	kJ/mol	Joback Method
hvap	79.06	kJ/mol	Joback Method
log10ws	-4.70		Estimated Solubility Method
log10ws	-4.72		Aqueous and cosolvent solubility data for drug-like organic compounds
log10ws	-4.70		Aqueous Solubility Prediction Method
logp	3.604		Crippen Method
mcvol	232.030	ml/mol	McGowan Method
pc	2108.07	kPa	Joback Method
rinpol	370.30		NIST Webbook
tb	818.00	K	Joback Method
tc	1041.45	K	Joback Method
tf	326.62	K	Thermodynamics of fenoxycarb in solution
tf	326.48	K	Aqueous Solubility Prediction Method
vc	0.867	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	680.09	J/mol×K	818.00	Joback Method
cpg	694.29	J/mol×K	855.24	Joback Method
cpg	707.23	J/mol×K	892.48	Joback Method
cpg	718.94	J/mol×K	929.73	Joback Method
cpg	729.41	J/mol×K	966.97	Joback Method
cpg	738.68	J/mol×K	1004.21	Joback Method
cpg	746.76	J/mol×K	1041.45	Joback Method

Sources

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

Estimated Solubility Method: http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

Aqueous and cosolvent solubility data for drug-like organic compounds: https://www.ncbi.nlm.nih.gov/pmc/articles/PMC2751500/

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C79127803&Units=SI

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

Thermodynamics of fenoxycarb in solution: https://www.doi.org/10.1016/j.jct.2013.06.007

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