Carbetamide

Other names:	(Phenylcarbamoyloxy)-2-N-ethylpropionamide
	(R)-N-Ethyl-2-(((phenylamino)carbonyl)oxy)propanamide
	1-(Ethylcarbamoyl)ethyl phenylcarbamate, (R)-
	11,561 RP
	11561RP
	2-Phenyl-carbamoyloxy-N-aethyl-propionamid
	Carbanilic acid, (1-ethylcarbamoyl)ethyl ester, D-(-)-
	Carbetamex
	Carbetamid
	Carbethamide
	D-(-)-1-(Ethylcarbamoyl)ethyl phenylcarbamate
	D-N-Ethylacetamide carbanilate
	D-N-Ethyllactamide carbanilate
	Lactamide, N-ethyl-, carbanilate (ester), D-
	Legurame
	Legurame PM
	N-Phenyl-1-(ethylcarbamoyl-1)-ethylcarbamate, D isomer
	Propanamide, N-ethyl-2-[[(phenylamino)carbonyl]oxy]-, (R)-
	RP 11561
	d-N-Ethyllactamide carbanilate (ester)
Inchi:	InChI=1S/C12H16N2O3/c1-3-13-11(15)9(2)17-12(16)14-10-7-5-4-6-8-10/h4-9H,3H2,1-2H
InchiKey:	AMRQXHFXNZFDCH-UHFFFAOYSA-N
Formula:	C12H16N2O3
SMILES:	CCNC(=O)C(C)OC(=O)Nc1ccccc1
Mol. weight [g/mol]:	236.27
CAS:	16118-49-3

Physical Properties

Property code	Value	Unit	Source
gf	-23.93	kJ/mol	Joback Method
hf	-310.20	kJ/mol	Joback Method
hfus	31.94	kJ/mol	Joback Method
hvap	72.97	kJ/mol	Joback Method
log10ws	-1.83		Estimated Solubility Method
log10ws	-1.83		Aqueous Solubility Prediction Method

logp	1.760		Crippen Method
mcvol	185.150	ml/mol	McGowan Method
pc	2781.78	kPa	Joback Method
tb	730.70	K	Joback Method
tc	946.62	K	Joback Method
tf	463.83	K	Joback Method
vc	0.694	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	514.90	J/mol×K	730.70	Joback Method
cpg	527.98	J/mol×K	766.69	Joback Method
cpg	540.10	J/mol×K	802.67	Joback Method
cpg	551.29	J/mol×K	838.66	Joback Method
cpg	561.57	J/mol×K	874.65	Joback Method
cpg	570.98	J/mol×K	910.63	Joback Method
cpg	579.54	J/mol×K	946.62	Joback Method

Sources

Estimated Solubility Method: http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C16118493&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method: https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume