Propanamide, N-ethyl-2-[[(phenylamino)carbonyl]oxy]-, (R)-

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
RP 11561
carbetamide
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

Physical Properties

Property code	Value	Unit	Source
hfus	31.94	kJ/mol	Joback Method
ie	8.34	eV	Cheméo Relay (1.0)
log10ws	-1.83		Aqueous Solubility Prediction Method
log10ws	-1.83		Estimated Solubility Method
logp	1.760		Crippen Method
mcvol	185.150	ml/mol	McGowan Method
tb	562.67	K	Cheméo Relay (1.0)

tf	382.87	K	Cheméo Relay (1.0)

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

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C16118493&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):

Legend

cpg: Ideal gas heat capacity
hfus: Enthalpy of fusion at standard conditions
ie: Ionization energy
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
tb: Normal Boiling Point Temperature
tf: Normal melting (fusion) point