Desmedipham

Other names:	3-(Aethoxycarbonylaminophenyl)-N-phenyl-carbamat
	3-Ethoxycarbonylaminophenyl N-phenylcarbamate
	Bentanex
	Betanal AM
	Betanex
	Carbamic acid, [3-[[(phenylamino)carbonyl]oxy]phenyl]-, ethyl ester
	Carbamic acid, phenylcarbamoyloxyphenyl-, ethyl ester
	Carbanilic acid, m-carbaniloyloxy-, ethyl ester
	Carbanilic acid, m-hydroxy-, ethyl ester, carbanilate (ester)
	EP 475
	Ethyl N-[3-(N-phenylcarbamoyloxy)phenyl]carbamate
	Ethyl [3-[[(phenylamino)carbonyl]oxy]phenylcarbamate
	Ethyl m-hydroxycarbanilate carbanilate
	Ethyl phenylcarbamoyloxyphenylcarbamate
	SN 38107
	Schering 38107
	Synbetan D
Inchi:	InChI=1S/C16H16N2O4/c1-2-21-15(19)18-13-9-6-10-14(11-13)22-16(20)17-12-7-4-3-5-8
InchiKey:	WZJZMXBKUWKXTQ-UHFFFAOYSA-N
Formula:	C16H16N2O4
SMILES:	CCOC(=O)Nc1cccc(OC(=O)Nc2ccccc2)c1
Mol. weight [g/mol]:	300.31
CAS:	13684-56-5

Physical Properties

Property code	Value	Unit	Source
gf	9.97	kJ/mol	Joback Method
hf	-294.64	kJ/mol	Joback Method
hfus	40.66	kJ/mol	Joback Method
hvap	87.61	kJ/mol	Joback Method
log10ws	-4.63		Estimated Solubility Method
log10ws	-4.63		Aqueous Solubility Prediction Method
logp	3.866		Crippen Method
mcvol	223.620	ml/mol	McGowan Method
pc	2527.73	kPa	Joback Method

tb	876.74	K	Joback Method
tc	1110.02	K	Joback Method
tf	394.81 ± 0.20	K	NIST Webbook
vc	0.834	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	706.75	J/mol×K	1071.14	Joback Method
cpg	661.26	J/mol×K	876.74	Joback Method
cpg	672.76	J/mol×K	915.62	Joback Method
cpg	683.02	J/mol×K	954.50	Joback Method
cpg	692.08	J/mol×K	993.38	Joback Method
cpg	699.98	J/mol×K	1032.26	Joback Method
cpg	712.41	J/mol×K	1110.02	Joback Method
hfust	32.75	kJ/mol	394.10	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C13684565&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
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

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
hfust: Enthalpy of fusion at a given temperature
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