Carbamic acid, (3-methylphenyl)-, 3-[(methoxycarbonyl)amino]phenyl ester

Other names: 3-(Carbomethoxyamino)phenyl 3-methylcarbanilate
3-(Methylphenyl)carbamic acid 3-((methoxycarbonyl)amino)phenyl ester
3-Methoxycarbonyl-N-(3'-methylphenyl)-carbamat
3-Methoxycarbonylaminophenyl N-3'-methylphenylcarbamate
3-[(Methoxycarbonyl)amino]phenyl (3-methylphenyl)carbamate
3-[(Methoxycarbonyl)amino]phenyl N-(3-methylphenyl)carbamate
Alegro
Beetomax
Beetup
Betanal
Betanal E
Betosip
Carbanilic acid, m-hydroxy-, methyl ester, m-methylcarbanilate
Carbanilic acid, m-hydroxy-, methyl ester, m-methylcarbanilate (ester)
EP-452
Fender
Fenmedifam
Gusto
Kemifam
Kemifam FL
Methyl 3-(m-tolylcarbamoyloxy)phenylcarbamate
Methyl N-[3-[N-(3-methylphenyl)carbamoyloxy]phenyl]carbamate
Methyl m-hydroxycarbanilate m-methylcarbanilate
Phenmedipham
Phenmediphame
Protrum K
SN 4075
SN-38584
Schering 4072
Schering-38584
Spin-aid
Synbetan P
Tripart beta
Vangard
m-Hydroxycarbanilic acid methyl ester m-methylcarbanilate

Inchi: InChI=1S/C16H16N2O4/c1-11-5-3-6-12(9-11)18-16(20)22-14-8-4-7-13(10-14)17-15(19)2

InchiKey: IDOWTHOLJBTAFI-UHFFFAOYSA-N

Formula: C16H16N2O4

SMILES: COC(=O)Nc1cccc(OC(=O)Nc2cccc(C)c2)c1

Mol. weight [g/mol]: 300.31

CAS: 13684-63-4

Physical Properties

Property code	Value	Unit	Source
gf	0.34	kJ/mol	Joback Method
hf	-306.11	kJ/mol	Joback Method
hfus	40.27	kJ/mol	Joback Method
hvap	88.27	kJ/mol	Joback Method
log10ws	-4.79		Aqueous Solubility Prediction Method
log10ws	-4.80		Estimated Solubility Method
logp	3.784		Crippen Method
mcvol	223.620	ml/mol	McGowan Method
pc	2490.03	kPa	Joback Method
tb	881.72	K	Joback Method
tc	1115.72	K	Joback Method
tf	423.90 ± 0.20	K	NIST Webbook
tf	424.48 ± 0.20	K	NIST Webbook
vc	0.834	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	659.70	J/mol×K	881.72	Joback Method
cpg	671.10	J/mol×K	920.72	Joback Method
cpg	681.26	J/mol×K	959.72	Joback Method
cpg	690.20	J/mol×K	998.72	Joback Method
cpg	697.94	J/mol×K	1037.72	Joback Method
cpg	704.52	J/mol×K	1076.72	Joback Method
cpg	709.96	J/mol×K	1115.72	Joback Method
hfust	39.62	kJ/mol	423.80	NIST Webbook
hfust	39.62	kJ/mol	423.80	NIST Webbook

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C13684634&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
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