Karbutilate

Other names:	Carbamic acid, (1,1-dimethylethyl)-, 3-[[(dimethylamino)carbonyl]amino]phenyl ester Carbamic acid, tert-butyl-, ester with 3-(m-hydroxyphenyl)-1,1-dimethylurea m-(3,3-Dimethylureido)phenyl tert-butylcarbamate Carbamic acid, tert-butyl-, m-(3,3-dimethylureido)phenyl ester NIA 11092 Tandex Tendex 3-(3,3-Dimethylureido)Phenyl tert-butylcarbamate 3-(3,3-Dimethylureido)phenyl N-tert-butylcarbamate m-(3,3-Dimethylharnstoff)-phenyl-tert-butylcarbamat tert-Butylcarbamic acid ester with 3-(m-hydroxyphenyl-1,1-dimethylurea tert-Butylcarbamic acid, ester of 3-(m-hydroxyphenyl)-1,1-dimethylurea FMC 11092 1,1-Dimethyl-3-(3-(N-tert-butylcarbamyloxy)phenyl)urea 3-(((Dimethylamino)carbonyl)amino)phenyl (1,1-dimethylethyl)carbamate Carbutilate Karbutylate 1,1-Dimethyl-3-[3-(N-tert-butylcarbamoyloxy)phenyl]urea NSC 222508
Inchi:	InChI=1S/C14H21N3O3/c1-14(2,3)16-13(19)20-11-8-6-7-10(9-11)15-12(18)17(4)5/h6-9H
InchiKey:	OWNAXTAAAQTBSP-UHFFFAOYSA-N
Formula:	C14H21N3O3
SMILES:	CN(C)C(=O)Nc1cccc(OC(=O)NC(C)(C)C)c1
Mol. weight [g/mol]:	279.33
CAS:	4849-32-5

Physical Properties

Property code	Value	Unit	Source
gf	99.34	kJ/mol	Joback Method
hf	-298.89	kJ/mol	Joback Method
hfus	35.86	kJ/mol	Joback Method
hvap	79.22	kJ/mol	Joback Method
log10ws	-3.49		Crippen Method
logp	2.667		Crippen Method
mcvol	223.310	ml/mol	McGowan Method
pc	2280.59	kPa	Joback Method
tb	791.09	K	Joback Method

tc	1006.33	K	Joback Method
tf	548.78	K	Joback Method
vc	0.819	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	663.15	J/mol×K	791.09	Joback Method
cpg	676.94	J/mol×K	826.96	Joback Method
cpg	689.69	J/mol×K	862.84	Joback Method
cpg	701.45	J/mol×K	898.71	Joback Method
cpg	712.28	J/mol×K	934.59	Joback Method
cpg	722.25	J/mol×K	970.46	Joback Method
cpg	731.41	J/mol×K	1006.33	Joback Method

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C4849325&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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