Carbamic acid, phenyl-, 1-methylethyl ester

Other names:

Carbanilic acid, isopropyl ester
Agermin
Birgin
Chem-Hoe
Collavin
Iso.PPC.
Isopropyl carbanilate
Isopropyl phenyl urethane
Isopropyl phenylcarbamate
Isopropyl phenylcarbmate
IFK
INPC
IPC
IPPC
Profam
Propham
Tixit
Tuberit
Tuberite
Y 2
Isopropyl N-phenylcarbamate
N-Phenylcarbamate d'isopropyle
O-Isopropyl N-phenylcarbamate
Ban-Hoe
Beet-Kleen
Isopropil-N-fenil-carbammato
Isopropyl carbanilic acid ester
Isopropyl-N-fenyl-carbamaat
Isopropyl-N-phenyl-carbamat
Isopropyl-N-phenylurethan
IFC
N-Phenyl isopropyl carbamate
N-Phenylcarbamic acid, isopropyl ester
Ortho grass killer
Phenylcarbamic acid,1-methylethyl ester
Prophame
Triherbide
Triherbide-IPC
USAF D-9
Isopropylester kyseliny karbanilove

	Premalox
	N-Phenyl-O-isopropylurethane
	Carbamate pesticide IPC
	1-Methylethyl phenylcarbamate
	ISO.PPC
	IsoPPC
	Carbamic acid, phenyl, isopropyl ester
	Carbamic acid, N-phenyl-, 1-methylethyl ester
Inchi:	InChI=1S/C10H13NO2/c1-8(2)13-10(12)11-9-6-4-3-5-7-9/h3-8H,1-2H3,(H,11,12)
InchiKey:	VXPLXMJHHKHSOA-UHFFFAOYSA-N
Formula:	C10H13NO2
SMILES:	CC(C)OC(=O)Nc1ccccc1
Mol. weight [g/mol]:	179.22
CAS:	122-42-9

Physical Properties

Property code	Value	Unit	Source
chs	-5351.00 ± 2.00	kJ/mol	NIST Webbook
gf	-1.24	kJ/mol	Joback Method
hf	-209.81	kJ/mol	Joback Method
hfus	20.06	kJ/mol	Joback Method
hvap	55.33	kJ/mol	Joback Method
log10ws	-2.69		Crippen Method
logp	2.643		Crippen Method
mcvol	145.420	ml/mol	McGowan Method
pc	3156.17	kPa	Joback Method
rinpol	1423.00		NIST Webbook
rinpol	1438.00		NIST Webbook
rinpol	1434.00		NIST Webbook
rinpol	1453.00		NIST Webbook
rinpol	1449.00		NIST Webbook
rinpol	1438.00		NIST Webbook
rinpol	1459.00		NIST Webbook
rinpol	1477.00		NIST Webbook
rinpol	1431.00		NIST Webbook
rinpol	1432.00		NIST Webbook
rinpol	1434.00		NIST Webbook
rinpol	1437.00		NIST Webbook
rinpol	1459.00		NIST Webbook
rinpol	1462.00		NIST Webbook

rinpol	1456.00		NIST Webbook
ripol	2000.00		NIST Webbook
tb	580.90	K	Joback Method
tc	798.13	K	Joback Method
tf	360.45 ± 0.20	K	NIST Webbook
tf	357.70 ± 0.20	K	NIST Webbook
vc	0.540	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	348.62	J/mol×K	580.90	Joback Method
cpg	362.53	J/mol×K	617.11	Joback Method
cpg	375.58	J/mol×K	653.31	Joback Method
cpg	387.80	J/mol×K	689.52	Joback Method
cpg	399.21	J/mol×K	725.72	Joback Method
cpg	409.83	J/mol×K	761.93	Joback Method
cpg	419.69	J/mol×K	798.13	Joback Method
hfust	19.37	kJ/mol	359.50	NIST Webbook
hfust	19.37	kJ/mol	359.50	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C122429&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method

Legend

chs: Standard solid enthalpy of combustion
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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume