Carbamic acid, methyl-, 3-methylphenyl ester

Other names:	3-Methylphenyl Methylcarbamate
	3-Methylphenyl N-methylcarbamate
	3-Tolyl N-methylcarbamate
	3-Tolyl methylcarbamate
	Carbamic acid, N-methyl-, 3-methylphenyl ester
	Carbamic acid, methyl-, 3-tolyl ester
	Carbamic acid, methyl-, m-tolyl ester
	DRC 3341
	Kumiai
	MTMC
	Metacrate
	Metholcarb
	Methylcarbamic acid m-tolyl ester
	Metolcarb
	NSC 91193
	S 1065
	Tsumacide
	Tsumaunka
	m-Cresyl N-methylcarbamate
	m-Cresyl ester of N-methylcarbamic acid
	m-Cresyl methylcarbamate
	m-Methylphenyl methylcarbamate
	m-Tolyl N-methylcarbamate
	m-Tolyl methylcarbamate
	m-Tolylester kyseliny methylkarbaminove
Inchi:	InChI=1S/C9H11NO2/c1-7-4-3-5-8(6-7)12-9(11)10-2/h3-6H,1-2H3,(H,10,11)
InchiKey:	VOEYXMAFNDNNED-UHFFFAOYSA-N
Formula:	C9H11NO2
SMILES:	CNC(=O)Oc1cccc(C)c1
Mol. weight [g/mol]:	165.19
CAS:	1129-41-5

Physical Properties

Property code	Value	Unit	Source
gf	-16.85	kJ/mol	Joback Method
hf	-195.36	kJ/mol	Joback Method

hfus	20.60	kJ/mol	Joback Method
hvap	54.16	kJ/mol	Joback Method
log10ws	-1.80		Aqueous Solubility Prediction Method
logp	1.713		Crippen Method
mcvol	131.330	ml/mol	McGowan Method
pc	3431.89	kPa	Joback Method
rinpol	1465.00		NIST Webbook
rinpol	1392.00		NIST Webbook
rinpol	1465.00		NIST Webbook
rinpol	1411.00		NIST Webbook
ripol	2048.00		NIST Webbook
tb	563.44	K	Joback Method
tc	780.85	K	Joback Method
tf	349.65	K	Aqueous Solubility Prediction Method
vc	0.490	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	301.19	J/mol×K	563.44	Joback Method
cpg	313.64	J/mol×K	599.68	Joback Method
cpg	325.37	J/mol×K	635.91	Joback Method
cpg	336.41	J/mol×K	672.15	Joback Method
cpg	346.75	J/mol×K	708.38	Joback Method
cpg	356.42	J/mol×K	744.62	Joback Method
cpg	365.43	J/mol×K	780.85	Joback Method

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1129415&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
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