Phenol, 3-methyl-5-(1-methylethyl)-, methylcarbamate

Other names: Carbamic acid, methyl-, m-cym-5-yl ester
Carbamult
m-Cym-5-yl methylcarbamate
EP 316
3-Isopropyl-5-Methylphenyl methylcarbamate
3-Isopropyl-5-methylphenyl N-methylcarbamate
ITC
3-Methyl-5-Isopropylphenyl methylcarbamate
3-Methyl-5-isopropylphenyl N-methylcarbamate
Minacide
Morton EP-316
Promecarb
Sch 34615
Schering 34615
Carbamic acid, N-methyl-, 3-methyl-5-isopropylphenyl ester
ENT 27,300-a
OMS 716
Promecarbe
Sn-316
SN 34615
UC 9880
NSC 35378
5-Isopropyl-m-tolyl methylcarbamate

Inchi: InChI=1S/C12H17NO2/c1-8(2)10-5-9(3)6-11(7-10)15-12(14)13-4/h5-8H,1-4H3,(H,13,14)

InchiKey: DTAPQAJKAFRNJB-UHFFFAOYSA-N

Formula: C12H16NO2

SMILES: CNC(=O)Oc1cc(C)cc(C(C)C)c1

Mol. weight [g/mol]: 206.26

CAS: 2631-37-0

Physical Properties

Property code	Value	Unit	Source
gf	-3.66	kJ/mol	Joback Method
hf	-274.03	kJ/mol	Joback Method
hfus	24.46	kJ/mol	Joback Method
hvap	61.11	kJ/mol	Joback Method

log10ws	-3.61		Crippen Method
logp	2.837		Crippen Method
mcvol	173.600	ml/mol	McGowan Method
pc	2495.01	kPa	Joback Method
rinpol	1695.00		NIST Webbook
rinpol	1689.00		NIST Webbook
tb	636.62	K	Joback Method
tc	848.49	K	Joback Method
tf	362.48 ± 0.20	K	NIST Webbook
vc	0.652	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	445.21	J/mol×K	636.62	Joback Method
cpg	460.01	J/mol×K	671.93	Joback Method
cpg	473.96	J/mol×K	707.24	Joback Method
cpg	487.07	J/mol×K	742.56	Joback Method
cpg	499.36	J/mol×K	777.87	Joback Method
cpg	510.85	J/mol×K	813.18	Joback Method
cpg	521.54	J/mol×K	848.49	Joback Method
hfust	23.04	kJ/mol	361.30	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2631370&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

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume