

Phenol, 3,4,5-trimethyl-, methylcarbamate

Other names:	Carbamic acid, methyl-, 3,4,5-trimethylphenyl ester Landrin Shell 8530 SD 8530 3,4,5-Landrin 3,4,5-Trimethylphenyl Methylcarbamate 3,4,5-Trimethylphenyl N-methylcarbamate ENT-25,843 Methylcarbamic acid 3,4,5-trimethylphenyl ester OMS-597 Shell sd-8530 3,4,5-Trimethylfenylester kyseliny methylkarbaminove Landrin-3,4,5
Inchi:	InChI=1S/C11H15NO2/c1-7-5-10(14-11(13)12-4)6-8(2)9(7)3/h5-6H,1-4H3,(H,12,13)
InchiKey:	AUQUAUIUNJIIEP-UHFFFAOYSA-N
Formula:	C11H15NO2
SMILES:	<chem>CNC(=O)Oc1cc(C)c(C)c(C)c1</chem>
Mol. weight [g/mol]:	193.24
CAS:	2686-99-9

Physical Properties

Property code	Value	Unit	Source
gf	-19.27	kJ/mol	Joback Method
hf	-259.58	kJ/mol	Joback Method
hfus	25.01	kJ/mol	Joback Method
hvap	59.93	kJ/mol	Joback Method
log10ws	-3.38		Crippen Method
logp	2.330		Crippen Method
mcvol	159.510	ml/mol	McGowan Method
pc	2687.42	kPa	Joback Method
tb	619.16	K	Joback Method
tc	831.23	K	Joback Method
tf	393.80 ± 0.20	K	NIST Webbook
vc	0.603	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	394.32	J/mol×K	619.16	Joback Method
cpg	407.94	J/mol×K	654.50	Joback Method
cpg	420.83	J/mol×K	689.85	Joback Method
cpg	433.00	J/mol×K	725.19	Joback Method
cpg	444.46	J/mol×K	760.54	Joback Method
cpg	455.20	J/mol×K	795.88	Joback Method
cpg	465.24	J/mol×K	831.23	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2686999&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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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