

Phenol, 2,3,5-trimethyl-, methylcarbamate

Other names:	Carbamic acid, methyl-, 2,3,5-trimethylphenyl ester SD 8786 2,3,5-Landrin 2,3,5-Trimethylphenyl Methylcarbamate Landrin B 2,3,5-Trimethylphenyl N-methylcarbamate
Inchi:	InChI=1S/C11H15NO2/c1-7-5-8(2)9(3)10(6-7)14-11(13)12-4/h5-6H,1-4H3,(H,12,13)
InchiKey:	NYOKZHDTNBDPOB-UHFFFAOYSA-N
Formula:	C11H15NO2
SMILES:	CNC(=O)Oc1cc(C)cc(C)c1C
Mol. weight [g/mol]:	193.24
CAS:	2655-15-4

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
rinpol	1666.00		NIST Webbook
tb	619.16	K	Joback Method
tc	831.23	K	Joback Method
tf	402.53	K	Joback Method
vc	0.603	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	394.32	J/molxK	619.16	Joback Method
cpg	407.94	J/molxK	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=C2655154&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
h vap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m cvol:	McGowan's characteristic volume
pc:	Critical Pressure
r inpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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