Carbamic acid, 2,4-dimethylphenyl, ethyl ester

Inchi: InChI=1S/C11H15NO2/c1-4-14-11(13)12-10-6-5-8(2)7-9(10)3/h5-7H,4H2,1-3H3,(H,12,13
InchiKey: DCVORZHXEUBUSJ-UHFFFAOYSA-N
Formula: C11H15NO2
SMILES: CCOC(O)=Nc1ccc(C)cc1C
Mol. weight [g/mol]: 193.24

Physical Properties

Property code	Value	Unit	Source
hf	-268.80	kJ/mol	Joback Method
hvap	66.16	kJ/mol	Joback Method
log10ws	-2.81		Crippen Method
logp	2.885		Crippen Method
mcvol	159.510	ml/mol	McGowan Method
pc	2505.01	kPa	Joback Method
rinpol	1544.00		NIST Webbook
rinpol	1547.00		NIST Webbook
rinpol	1550.00		NIST Webbook
rinpol	1544.00		NIST Webbook
tb	678.88	K	Joback Method
tc	886.42	K	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R37713&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

hf:	Enthalpy of formation 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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

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