Carbamic acid, phenyl-, octyl ester

Other names: Carbanilic acid, n-octyl ester
Inchi: InChI=1S/C15H23NO2/c1-2-3-4-5-6-10-13-18-15(17)16-14-11-8-7-9-12-14/h7-9,11-12H,
InchiKey: PPGXIFWHXQZPKV-UHFFFAOYSA-N
Formula: C15H23NO2
SMILES: CCCCCCCCOC(O)=Nc1ccccc1
Mol. weight [g/mol]: 249.35
CAS: 6327-52-2

Physical Properties

Property code	Value	Unit	Source
hf	-328.42	kJ/mol	Joback Method
hvap	73.74	kJ/mol	Joback Method
log10ws	-4.37		Crippen Method
logp	4.609		Crippen Method
mcvol	215.870	ml/mol	McGowan Method
pc	1807.70	kPa	Joback Method
tb	760.44	K	Joback Method
tc	958.35	K	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C6327522&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

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature