

Carbamic acid, phenyl-, dodecyl ester

Other names:	Carbanilic acid, n-dodecyl ester
Inchi:	InChI=1S/C19H31NO2/c1-2-3-4-5-6-7-8-9-10-14-17-22-19(21)20-18-15-12-11-13-16-18/
InchiKey:	UATVIVWPWXCCFM-UHFFFAOYSA-N
Formula:	C19H31NO2
SMILES:	CCCCCCCCCCCCOC(=O)Nc1ccccc1
Mol. weight [g/mol]:	305.45
CAS:	5796-07-6

Physical Properties

Property code	Value	Unit	Source
gf	76.98	kJ/mol	Joback Method
hf	-390.29	kJ/mol	Joback Method
hfus	46.89	kJ/mol	Joback Method
hvap	75.76	kJ/mol	Joback Method
log10ws	-6.34		Crippen Method
logp	6.156		Crippen Method
mcvol	272.230	ml/mol	McGowan Method
pc	1421.85	kPa	Joback Method
tb	787.26	K	Joback Method
tc	981.39	K	Joback Method
tf	455.13	K	Joback Method
vc	1.050	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	829.80	J/molxK	787.26	Joback Method
cpg	847.10	J/molxK	819.61	Joback Method
cpg	863.35	J/molxK	851.97	Joback Method
cpg	878.60	J/molxK	884.32	Joback Method
cpg	892.88	J/molxK	916.68	Joback Method
cpg	906.22	J/molxK	949.03	Joback Method
cpg	918.67	J/molxK	981.39	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5796076&Units=SI

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
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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