

Carbanilic acid, n-undecyl ester

Inchi:	InChI=1S/C18H29NO2/c1-2-3-4-5-6-7-8-9-13-16-21-18(20)19-17-14-11-10-12-15-17/h10
InchiKey:	GWMSSZJEBQKCFD-UHFFFAOYSA-N
Formula:	C18H29NO2
SMILES:	CCCCCCCCCOC(=O)Nc1ccccc1
Mol. weight [g/mol]:	291.43
CAS:	110273-47-7

Physical Properties

Property code	Value	Unit	Source
gf	68.56	kJ/mol	Joback Method
hf	-369.65	kJ/mol	Joback Method
hfus	44.30	kJ/mol	Joback Method
hvap	73.53	kJ/mol	Joback Method
log10ws	-5.93		Crippen Method
logp	5.766		Crippen Method
mcvol	258.140	ml/mol	McGowan Method
pc	1530.66	kPa	Joback Method
tb	764.38	K	Joback Method
tc	958.76	K	Joback Method
tf	443.86	K	Joback Method
vc	0.995	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	771.67	J/molxK	764.38	Joback Method
cpg	788.73	J/molxK	796.78	Joback Method
cpg	804.76	J/molxK	829.17	Joback Method
cpg	819.81	J/molxK	861.57	Joback Method
cpg	833.91	J/molxK	893.96	Joback Method
cpg	847.09	J/molxK	926.36	Joback Method
cpg	859.40	J/molxK	958.76	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C110273477&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
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccvol:	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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