

M-nitro carbanilic acid, n-undecyl ester

Inchi:	InChI=1S/C18H28N2O4/c1-2-3-4-5-6-7-8-9-10-14-24-18(21)19-16-12-11-13-17(15-16)20
InchiKey:	ARGNOEPEIHBMJT-UHFFFAOYSA-N
Formula:	C18H28N2O4
SMILES:	CCCCCCCCCOC(=O)Nc1cccc([N+](=O)[O-])c1
Mol. weight [g/mol]:	336.43
CAS:	95126-58-2

Physical Properties

Property code	Value	Unit	Source
gf	94.48	kJ/mol	Joback Method
hf	-391.88	kJ/mol	Joback Method
hfus	55.27	kJ/mol	Joback Method
hvap	90.78	kJ/mol	Joback Method
log10ws	-6.58		Crippen Method
logp	5.674		Crippen Method
mvol	275.560	ml/mol	McGowan Method
pc	1527.07	kPa	Joback Method
tb	921.20	K	Joback Method
tc	1139.10	K	Joback Method
tf	599.99	K	Joback Method
vc	1.077	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	887.94	J/molxK	921.20	Joback Method
cpg	902.01	J/molxK	957.52	Joback Method
cpg	914.95	J/molxK	993.83	Joback Method
cpg	926.81	J/molxK	1030.15	Joback Method
cpg	937.64	J/molxK	1066.47	Joback Method
cpg	947.49	J/molxK	1102.79	Joback Method
cpg	956.40	J/molxK	1139.10	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C95126582&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

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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