P-nitro carbanilic acid, n-undecyl ester

Inchi: InChI=1S/C18H28N2O4/c1-2-3-4-5-6-7-8-9-10-15-24-18(21)19-16-11-13-17(14-12-16)20
InchiKey: NQKPOXVRXBGLGC-UHFFFAOYSA-N
Formula: C18H28N2O4
SMILES: CCCCCCCCCCCOC(=O)Nc1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]: 336.43
CAS: 93999-89-4

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
mcvol	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/mol×K	921.20	Joback Method
cpg	902.01	J/mol×K	957.52	Joback Method
cpg	914.95	J/mol×K	993.83	Joback Method
cpg	926.81	J/mol×K	1030.15	Joback Method
cpg	937.64	J/mol×K	1066.47	Joback Method
cpg	947.49	J/mol×K	1102.79	Joback Method
cpg	956.40	J/mol×K	1139.10	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C93999894&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
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume