4-Nitrobenzoic acid, undecyl ester

Other names: undecyl 4-nitrobenzoate
Inchi: InChI=1S/C18H27NO4/c1-2-3-4-5-6-7-8-9-10-15-23-18(20)16-11-13-17(14-12-16)19(21)
InchiKey: LBXQBIXFFOGQIH-UHFFFAOYSA-N
Formula: C18H27NO4
SMILES: CCCCCCCCCCCOC(=O)c1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]: 321.41
CAS: 93094-34-9

Physical Properties

Property code	Value	Unit	Source
gf	5.09	kJ/mol	Joback Method
hf	-445.35	kJ/mol	Joback Method
hfus	50.18	kJ/mol	Joback Method
hvap	84.35	kJ/mol	Joback Method
log10ws	-6.55		Crippen Method
logp	5.282		Crippen Method
mcvol	265.580	ml/mol	McGowan Method
pc	1511.67	kPa	Joback Method
rinpol	2443.00		NIST Webbook
rinpol	2408.00		NIST Webbook
rinpol	2444.00		NIST Webbook
rinpol	2421.00		NIST Webbook
rinpol	2443.00		NIST Webbook
rinpol	2408.00		NIST Webbook
rinpol	2435.00		NIST Webbook
ripol	3185.00		NIST Webbook
ripol	3235.00		NIST Webbook
ripol	3185.00		NIST Webbook
ripol	3235.00		NIST Webbook
ripol	3235.00		NIST Webbook
ripol	3220.00		NIST Webbook
tb	871.03	K	Joback Method
tc	1085.36	K	Joback Method
tf	547.33	K	Joback Method
vc	1.042	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	831.32	J/mol×K	871.03	Joback Method
cpg	846.26	J/mol×K	906.75	Joback Method
cpg	860.09	J/mol×K	942.47	Joback Method
cpg	872.86	J/mol×K	978.20	Joback Method
cpg	884.61	J/mol×K	1013.92	Joback Method
cpg	895.38	J/mol×K	1049.64	Joback Method
cpg	905.22	J/mol×K	1085.36	Joback Method

Sources

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=C93094349&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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