Nonanoic acid, 4-nitrophenyl ester

Other names: Nonoic acid, 4-nitrophenyl ester
Inchi: InChI=1S/C15H21NO4/c1-2-3-4-5-6-7-8-15(17)20-14-11-9-13(10-12-14)16(18)19/h9-12H
InchiKey: TZQXKOGMKYABTL-UHFFFAOYSA-N
Formula: C15H21NO4
SMILES: CCCCCCCCC(=O)Oc1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]: 279.33

Physical Properties

Property code	Value	Unit	Source
gf	-20.17	kJ/mol	Joback Method
hf	-383.43	kJ/mol	Joback Method
hfus	42.41	kJ/mol	Joback Method
hvap	77.67	kJ/mol	Joback Method
log10ws	-5.37		Crippen Method
logp	4.251		Crippen Method
mcvol	223.310	ml/mol	McGowan Method
pc	1916.94	kPa	Joback Method
rinpol	2239.00		NIST Webbook
rinpol	2239.00		NIST Webbook
tb	802.39	K	Joback Method
tc	1021.16	K	Joback Method
tf	513.52	K	Joback Method
vc	0.874	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	660.01	J/mol×K	802.39	Joback Method
cpg	674.29	J/mol×K	838.85	Joback Method
cpg	687.53	J/mol×K	875.31	Joback Method
cpg	699.75	J/mol×K	911.78	Joback Method
cpg	711.01	J/mol×K	948.24	Joback Method
cpg	721.32	J/mol×K	984.70	Joback Method
cpg	730.73	J/mol×K	1021.16	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=U358028&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume