2-Heptenoic acid, 4-nitrophenyl ester

Inchi: InChI=1S/C13H15NO4/c1-2-3-4-5-6-13(15)18-12-9-7-11(8-10-12)14(16)17/h5-10H,2-4H2
InchiKey: HIKWTNDLAGMQDA-AATRIKPKSA-N
Formula: C13H15NO4
SMILES: CCCCC=CC(=O)Oc1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]: 249.26

Physical Properties

Property code	Value	Unit	Source
gf	43.21	kJ/mol	Joback Method
hf	-224.93	kJ/mol	Joback Method
hfus	37.43	kJ/mol	Joback Method
hvap	73.18	kJ/mol	Joback Method
log10ws	-4.38		Crippen Method
logp	3.247		Crippen Method
mcvol	190.830	ml/mol	McGowan Method
pc	2402.92	kPa	Joback Method
rinpol	2089.00		NIST Webbook
rinpol	2089.00		NIST Webbook
tb	760.79	K	Joback Method
tc	993.55	K	Joback Method
tf	485.90	K	Joback Method
vc	0.742	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	525.56	J/mol×K	760.79	Joback Method
cpg	538.62	J/mol×K	799.58	Joback Method
cpg	550.70	J/mol×K	838.38	Joback Method
cpg	561.86	J/mol×K	877.17	Joback Method
cpg	572.13	J/mol×K	915.96	Joback Method
cpg	581.57	J/mol×K	954.76	Joback Method
cpg	590.24	J/mol×K	993.55	Joback Method

Sources

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=U406906&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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