4-Nitrophenyl caprylate

Other names: Octanoic acid, 4-nitrophenyl ester
Inchi: InChI=1S/C14H19NO4/c1-2-3-4-5-6-7-14(16)19-13-10-8-12(9-11-13)15(17)18/h8-11H,2-
InchiKey: GGIDEJQGAZSTES-UHFFFAOYSA-N
Formula: C14H19NO4
SMILES: CCCCCCCC(=O)Oc1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]: 265.31
CAS: 1956-10-1

Physical Properties

Property code	Value	Unit	Source
gf	-28.59	kJ/mol	Joback Method
hf	-362.79	kJ/mol	Joback Method
hfus	39.82	kJ/mol	Joback Method
hvap	75.44	kJ/mol	Joback Method
log10ws	-4.95		Crippen Method
logp	3.861		Crippen Method
mcvol	209.220	ml/mol	McGowan Method
pc	2088.84	kPa	Joback Method
rinpol	2063.00		NIST Webbook
rinpol	2063.00		NIST Webbook
tb	779.51	K	Joback Method
tc	1000.99	K	Joback Method
tf	502.25	K	Joback Method
vc	0.818	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	604.78	J/mol×K	779.51	Joback Method
cpg	618.77	J/mol×K	816.42	Joback Method
cpg	631.73	J/mol×K	853.34	Joback Method
cpg	643.71	J/mol×K	890.25	Joback Method
cpg	654.73	J/mol×K	927.16	Joback Method
cpg	664.82	J/mol×K	964.07	Joback Method

cpg	674.02	J/mol×K	1000.99	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=C1956101&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