Hexadecanoic acid, 4-nitrophenyl ester

Other names: 4-nitrophenyl palmitate
Inchi: InChI=1S/C22H35NO4/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-22(24)27-21-18-16-20(17-
InchiKey: LVZSQWIWCANHPF-UHFFFAOYSA-N
Formula: C22H35NO4
SMILES: CCCCCCCCCCCCCCCC(=O)Oc1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]: 377.52
CAS: 1492-30-4

Physical Properties

Property code	Value	Unit	Source
gf	38.77	kJ/mol	Joback Method
hf	-527.91	kJ/mol	Joback Method
hfus	60.54	kJ/mol	Joback Method
hvap	93.25	kJ/mol	Joback Method
log10ws	-8.30		Crippen Method
logp	6.982		Crippen Method
mcvol	321.940	ml/mol	McGowan Method
pc	1144.44	kPa	Joback Method
tb	962.55	K	Joback Method
tc	1181.22	K	Joback Method
tf	592.41	K	Joback Method
vc	1.266	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1070.37	J/mol×K	962.55	Joback Method
cpg	1086.10	J/mol×K	998.99	Joback Method
cpg	1100.59	J/mol×K	1035.44	Joback Method
cpg	1113.90	J/mol×K	1071.88	Joback Method
cpg	1126.10	J/mol×K	1108.33	Joback Method
cpg	1137.25	J/mol×K	1144.77	Joback Method
cpg	1147.40	J/mol×K	1181.22	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=C1492304&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume