Pimelic acid, 4-methyl-2-pentyl 3-nitrophenyl ester

Inchi: InChI=1S/C19H27NO6/c1-14(2)12-15(3)25-18(21)10-5-4-6-11-19(22)26-17-9-7-8-16(13-
InchiKey: FBJAVPKJLAJDDZ-UHFFFAOYSA-N
Formula: C19H27NO6
SMILES: CC(C)CC(C)OC(=O)CCCCCC(=O)Oc1cccc([N+](=O)[O-])c1
Mol. weight [g/mol]: 365.42

Physical Properties

Property code	Value	Unit	Source
gf	-225.29	kJ/mol	Joback Method
hf	-721.35	kJ/mol	Joback Method
hfus	48.51	kJ/mol	Joback Method
hvap	94.95	kJ/mol	Joback Method
log10ws	-5.77		Crippen Method
logp	4.428		Crippen Method
mcvol	287.110	ml/mol	McGowan Method
pc	1472.49	kPa	Joback Method
rinpol	2677.00		NIST Webbook
rinpol	2677.00		NIST Webbook
tb	969.32	K	Joback Method
tc	1195.93	K	Joback Method
tf	600.76	K	Joback Method
vc	1.109	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	930.05	J/mol×K	969.32	Joback Method
cpg	942.58	J/mol×K	1007.09	Joback Method
cpg	953.75	J/mol×K	1044.86	Joback Method
cpg	963.59	J/mol×K	1082.62	Joback Method
cpg	972.14	J/mol×K	1120.39	Joback Method
cpg	979.43	J/mol×K	1158.16	Joback Method
cpg	985.50	J/mol×K	1195.93	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U416754&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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