Pimelic acid, 3-nitrophenyl pentyl ester

Inchi: InChI=1S/C18H25NO6/c1-2-3-7-13-24-17(20)11-5-4-6-12-18(21)25-16-10-8-9-15(14-16)
InchiKey: ZFAHBTLYYIPAJA-UHFFFAOYSA-N
Formula: C18H25NO6
SMILES: CCCCCOC(=O)CCCCCC(=O)Oc1cccc([N+](=O)[O-])c1
Mol. weight [g/mol]: 351.39

Physical Properties

Property code	Value	Unit	Source
gf	-228.83	kJ/mol	Joback Method
hf	-690.15	kJ/mol	Joback Method
hfus	52.96	kJ/mol	Joback Method
hvap	93.50	kJ/mol	Joback Method
log10ws	-5.48		Crippen Method
logp	4.184		Crippen Method
mcvol	273.020	ml/mol	McGowan Method
pc	1567.23	kPa	Joback Method
rinpol	2722.00		NIST Webbook
rinpol	2722.00		NIST Webbook
tb	947.32	K	Joback Method
tc	1169.79	K	Joback Method
tf	619.49	K	Joback Method
vc	1.065	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	870.47	J/mol×K	947.32	Joback Method
cpg	882.84	J/mol×K	984.40	Joback Method
cpg	893.96	J/mol×K	1021.48	Joback Method
cpg	903.85	J/mol×K	1058.56	Joback Method
cpg	912.55	J/mol×K	1095.64	Joback Method
cpg	920.08	J/mol×K	1132.72	Joback Method
cpg	926.47	J/mol×K	1169.79	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U416755&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

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