Pimelic acid, heptyl 3-nitrophenyl ester

Inchi: InChI=1S/C20H29NO6/c1-2-3-4-5-9-15-26-19(22)13-7-6-8-14-20(23)27-18-12-10-11-17(
InchiKey: UCLZLQUFVNEQDX-UHFFFAOYSA-N
Formula: C20H29NO6
SMILES: CCCCCCCOC(=O)CCCCCC(=O)Oc1cccc([N+](=O)[O-])c1
Mol. weight [g/mol]: 379.45

Physical Properties

Property code	Value	Unit	Source
gf	-211.99	kJ/mol	Joback Method
hf	-731.43	kJ/mol	Joback Method
hfus	58.14	kJ/mol	Joback Method
hvap	97.95	kJ/mol	Joback Method
log10ws	-6.32		Crippen Method
logp	4.964		Crippen Method
mcvol	301.200	ml/mol	McGowan Method
pc	1353.63	kPa	Joback Method
rinpol	2931.00		NIST Webbook
rinpol	2931.00		NIST Webbook
tb	993.08	K	Joback Method
tc	1218.94	K	Joback Method
tf	642.03	K	Joback Method
vc	1.177	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	988.43	J/mol×K	993.08	Joback Method
cpg	1001.03	J/mol×K	1030.72	Joback Method
cpg	1012.27	J/mol×K	1068.37	Joback Method
cpg	1022.20	J/mol×K	1106.01	Joback Method
cpg	1030.85	J/mol×K	1143.65	Joback Method
cpg	1038.27	J/mol×K	1181.30	Joback Method
cpg	1044.48	J/mol×K	1218.94	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=U416757&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