Pimelic acid, ethyl 3-nitrophenyl ester

Inchi: InChI=1S/C15H19NO6/c1-2-21-14(17)9-4-3-5-10-15(18)22-13-8-6-7-12(11-13)16(19)20/
InchiKey: CSNYEEIHPWWQJL-UHFFFAOYSA-N
Formula: C15H19NO6
SMILES: CCOC(=O)CCCCCC(=O)Oc1cccc([N+](=O)[O-])c1
Mol. weight [g/mol]: 309.31

Physical Properties

Property code	Value	Unit	Source
gf	-254.09	kJ/mol	Joback Method
hf	-628.23	kJ/mol	Joback Method
hfus	45.19	kJ/mol	Joback Method
hvap	86.82	kJ/mol	Joback Method
log10ws	-4.23		Crippen Method
logp	3.014		Crippen Method
mcvol	230.750	ml/mol	McGowan Method
pc	1996.55	kPa	Joback Method
rinpol	2423.00		NIST Webbook
rinpol	2423.00		NIST Webbook
tb	878.68	K	Joback Method
tc	1102.32	K	Joback Method
tf	585.68	K	Joback Method
vc	0.897	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	698.25	J/mol×K	878.68	Joback Method
cpg	710.17	J/mol×K	915.95	Joback Method
cpg	720.95	J/mol×K	953.23	Joback Method
cpg	730.61	J/mol×K	990.50	Joback Method
cpg	739.17	J/mol×K	1027.77	Joback Method
cpg	746.64	J/mol×K	1065.04	Joback Method
cpg	753.04	J/mol×K	1102.32	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U416750&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