Pimelic acid, isobutyl 3-nitrophenyl ester

Inchi: InChI=1S/C17H23NO6/c1-13(2)12-23-16(19)9-4-3-5-10-17(20)24-15-8-6-7-14(11-15)18(
InchiKey: BTAUBYUDJMLXLL-UHFFFAOYSA-N
Formula: C17H23NO6
SMILES: CC(C)COC(=O)CCCCCC(=O)Oc1cccc([N+](=O)[O-])c1
Mol. weight [g/mol]: 337.37

Physical Properties

Property code	Value	Unit	Source
gf	-239.69	kJ/mol	Joback Method
hf	-674.79	kJ/mol	Joback Method
hfus	46.85	kJ/mol	Joback Method
hvap	90.89	kJ/mol	Joback Method
log10ws	-4.82		Crippen Method
logp	3.650		Crippen Method
mcvol	258.930	ml/mol	McGowan Method
pc	1704.71	kPa	Joback Method
rinpol	2582.00		NIST Webbook
rinpol	2582.00		NIST Webbook
tb	924.00	K	Joback Method
tc	1148.18	K	Joback Method
tf	593.22	K	Joback Method
vc	1.004	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	812.88	J/mol×K	924.00	Joback Method
cpg	825.20	J/mol×K	961.36	Joback Method
cpg	836.26	J/mol×K	998.73	Joback Method
cpg	846.10	J/mol×K	1036.09	Joback Method
cpg	854.75	J/mol×K	1073.45	Joback Method
cpg	862.23	J/mol×K	1110.82	Joback Method
cpg	868.56	J/mol×K	1148.18	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U416752&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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