Pimelic acid, butyl 2-nitrophenyl ester

Inchi: InChI=1S/C17H23NO6/c1-2-3-13-23-16(19)11-5-4-6-12-17(20)24-15-10-8-7-9-14(15)18(
InchiKey: XONQJJINSZLYFP-UHFFFAOYSA-N
Formula: C17H23NO6
SMILES: CCCCOC(=O)CCCCCC(=O)Oc1ccccc1[N+](=O)[O-]
Mol. weight [g/mol]: 337.37

Physical Properties

Property code	Value	Unit	Source
gf	-237.25	kJ/mol	Joback Method
hf	-669.51	kJ/mol	Joback Method
hfus	50.37	kJ/mol	Joback Method
hvap	91.28	kJ/mol	Joback Method
log10ws	-5.07		Crippen Method
logp	3.794		Crippen Method
mcvol	258.930	ml/mol	McGowan Method
pc	1693.51	kPa	Joback Method
rinpol	2528.00		NIST Webbook
rinpol	2528.00		NIST Webbook
tb	924.44	K	Joback Method
tc	1146.52	K	Joback Method
tf	608.22	K	Joback Method
vc	1.010	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	812.38	J/mol×K	924.44	Joback Method
cpg	824.62	J/mol×K	961.45	Joback Method
cpg	835.65	J/mol×K	998.47	Joback Method
cpg	845.49	J/mol×K	1035.48	Joback Method
cpg	854.17	J/mol×K	1072.49	Joback Method
cpg	861.72	J/mol×K	1109.51	Joback Method
cpg	868.15	J/mol×K	1146.52	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U416744&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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