Glutaric acid, isobutyl 2-(4-nitrophenoxy)ethyl ester

Inchi: InChI=1S/C17H23NO7/c1-13(2)12-25-17(20)5-3-4-16(19)24-11-10-23-15-8-6-14(7-9-15)
InchiKey: ILMMPEMFRRYAJI-UHFFFAOYSA-N
Formula: C17H23NO7
SMILES: CC(C)COC(=O)CCCC(=O)OCCOc1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]: 353.37

Physical Properties

Property code	Value	Unit	Source
gf	-344.69	kJ/mol	Joback Method
hf	-807.01	kJ/mol	Joback Method
hfus	48.04	kJ/mol	Joback Method
hvap	93.30	kJ/mol	Joback Method
log10ws	-3.91		Crippen Method
logp	2.886		Crippen Method
mcvol	264.800	ml/mol	McGowan Method
pc	1681.03	kPa	Joback Method
rinpol	2763.00		NIST Webbook
tb	946.42	K	Joback Method
tc	1171.08	K	Joback Method
tf	615.45	K	Joback Method
vc	1.022	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	839.08	J/mol×K	946.42	Joback Method
cpg	850.58	J/mol×K	983.86	Joback Method
cpg	860.71	J/mol×K	1021.31	Joback Method
cpg	869.46	J/mol×K	1058.75	Joback Method
cpg	876.86	J/mol×K	1096.20	Joback Method
cpg	882.89	J/mol×K	1133.64	Joback Method
cpg	887.59	J/mol×K	1171.08	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U376794&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