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

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

Physical Properties

Property code	Value	Unit	Source
gf	-342.25	kJ/mol	Joback Method
hf	-801.73	kJ/mol	Joback Method
hfus	51.56	kJ/mol	Joback Method
hvap	93.69	kJ/mol	Joback Method
log10ws	-4.15		Crippen Method
logp	3.030		Crippen Method
mcvol	264.800	ml/mol	McGowan Method
pc	1670.06	kPa	Joback Method
rinpol	2811.00		NIST Webbook
rinpol	2811.00		NIST Webbook
tb	946.86	K	Joback Method
tc	1169.74	K	Joback Method
tf	630.45	K	Joback Method
vc	1.028	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	838.59	J/mol×K	946.86	Joback Method
cpg	850.06	J/mol×K	984.01	Joback Method
cpg	860.18	J/mol×K	1021.15	Joback Method
cpg	868.96	J/mol×K	1058.30	Joback Method
cpg	876.42	J/mol×K	1095.45	Joback Method
cpg	882.55	J/mol×K	1132.59	Joback Method
cpg	887.38	J/mol×K	1169.74	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U376795&Units=SI

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

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