Glutaric acid, 2-methylpent-3-yl 4-nitrophenyl ester

Inchi: InChI=1S/C17H23NO6/c1-4-15(12(2)3)24-17(20)7-5-6-16(19)23-14-10-8-13(9-11-14)18(

InchiKey: WQZSQZMUZKYHHM-UHFFFAOYSA-N

Formula: C17H23NO6

SMILES: CCC(OC(=O)CCCC(=O)Oc1ccc([N+](=O)[O-])cc1)C(C)C

Mol. weight [g/mol]: 337.37

Physical Properties

Property code	Value	Unit	Source
gf	-242.13	kJ/mol	Joback Method
hf	-680.07	kJ/mol	Joback Method
hfus	43.33	kJ/mol	Joback Method
hvap	90.50	kJ/mol	Joback Method
log10ws	-4.94		Crippen Method
logp	3.648		Crippen Method
mcvol	258.930	ml/mol	McGowan Method
pc	1716.03	kPa	Joback Method
rinpol	2474.00		NIST Webbook
rinpol	2474.00		NIST Webbook
tb	923.56	K	Joback Method
tc	1150.00	K	Joback Method
tf	578.22	K	Joback Method
vc	0.998	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	813.39	J/mol×K	923.56	Joback Method
cpg	825.78	J/mol×K	961.30	Joback Method
cpg	836.89	J/mol×K	999.04	Joback Method
cpg	846.73	J/mol×K	1036.78	Joback Method
cpg	855.34	J/mol×K	1074.52	Joback Method
cpg	862.75	J/mol×K	1112.26	Joback Method
cpg	868.97	J/mol×K	1150.00	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=U391971&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