Glutaric acid, 2-methylhex-3-yl 2-(2-nitrophenyl)ethyl ester

Inchi: InChI=1S/C20H29NO6/c1-4-8-18(15(2)3)27-20(23)12-7-11-19(22)26-14-13-16-9-5-6-10-
InchiKey: LABUEBFFQUWBLX-UHFFFAOYSA-N
Formula: C20H29NO6
SMILES: CCCC(OC(=O)CCCC(=O)OCCc1ccccc1[N+](=O)[O-])C(C)C
Mol. weight [g/mol]: 379.45

Physical Properties

Property code	Value	Unit	Source
gf	-216.87	kJ/mol	Joback Method
hf	-741.99	kJ/mol	Joback Method
hfus	51.10	kJ/mol	Joback Method
hvap	97.18	kJ/mol	Joback Method
log10ws	-5.54		Crippen Method
logp	4.219		Crippen Method
mcvol	301.200	ml/mol	McGowan Method
pc	1369.71	kPa	Joback Method
rinpol	2747.00		NIST Webbook
tb	992.20	K	Joback Method
tc	1220.18	K	Joback Method
tf	612.03	K	Joback Method
vc	1.165	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	989.23	J/mol×K	992.20	Joback Method
cpg	1001.81	J/mol×K	1030.20	Joback Method
cpg	1012.99	J/mol×K	1068.19	Joback Method
cpg	1022.80	J/mol×K	1106.19	Joback Method
cpg	1031.27	J/mol×K	1144.19	Joback Method
cpg	1038.46	J/mol×K	1182.18	Joback Method
cpg	1044.40	J/mol×K	1220.18	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=U377524&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