Glutaric acid, hexyl 2-(2-nitrophenyl)ethyl ester

Inchi: InChI=1S/C19H27NO6/c1-2-3-4-7-14-25-18(21)11-8-12-19(22)26-15-13-16-9-5-6-10-17(
InchiKey: GBXPQDMZOZUQDE-UHFFFAOYSA-N
Formula: C19H27NO6
SMILES: CCCCCCOC(=O)CCCC(=O)OCCc1ccccc1[N+](=O)[O-]
Mol. weight [g/mol]: 365.42

Physical Properties

Property code	Value	Unit	Source
gf	-220.41	kJ/mol	Joback Method
hf	-710.79	kJ/mol	Joback Method
hfus	55.55	kJ/mol	Joback Method
hvap	95.73	kJ/mol	Joback Method
log10ws	-5.25		Crippen Method
logp	3.974		Crippen Method
mcvol	287.110	ml/mol	McGowan Method
pc	1454.57	kPa	Joback Method
rinpol	2793.00		NIST Webbook
tb	970.20	K	Joback Method
tc	1193.92	K	Joback Method
tf	630.76	K	Joback Method
vc	1.121	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	929.17	J/mol×K	970.20	Joback Method
cpg	941.66	J/mol×K	1007.49	Joback Method
cpg	952.85	J/mol×K	1044.77	Joback Method
cpg	962.77	J/mol×K	1082.06	Joback Method
cpg	971.45	J/mol×K	1119.34	Joback Method
cpg	978.94	J/mol×K	1156.63	Joback Method
cpg	985.26	J/mol×K	1193.92	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=U377525&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