Glutaric acid, hexyl 3-methyl-2-nitrobenzyl ester

Inchi: InChI=1S/C19H27NO6/c1-3-4-5-6-13-25-17(21)11-8-12-18(22)26-14-16-10-7-9-15(2)19(
InchiKey: LHUQAAOUVCQVIT-UHFFFAOYSA-N
Formula: C19H27NO6
SMILES: CCCCCCOC(=O)CCCC(=O)OCc1cccc(C)c1[N+](=O)[O-]
Mol. weight [g/mol]: 365.42

Physical Properties

Property code	Value	Unit	Source
gf	-230.04	kJ/mol	Joback Method
hf	-722.26	kJ/mol	Joback Method
hfus	55.16	kJ/mol	Joback Method
hvap	96.39	kJ/mol	Joback Method
log10ws	-5.81		Crippen Method
logp	4.240		Crippen Method
mcvol	287.110	ml/mol	McGowan Method
pc	1438.07	kPa	Joback Method
rinpol	2678.00		NIST Webbook
tb	975.18	K	Joback Method
tc	1199.80	K	Joback Method
tf	643.28	K	Joback Method
vc	1.121	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	927.88	J/mol×K	975.18	Joback Method
cpg	940.23	J/mol×K	1012.62	Joback Method
cpg	951.26	J/mol×K	1050.05	Joback Method
cpg	960.98	J/mol×K	1087.49	Joback Method
cpg	969.43	J/mol×K	1124.93	Joback Method
cpg	976.62	J/mol×K	1162.36	Joback Method
cpg	982.59	J/mol×K	1199.80	Joback Method

Sources

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=U376736&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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