Glutaric acid, 2-methylhex-3-yl 3-methyl-2-nitrobenzyl ester

Inchi: InChI=1S/C20H29NO6/c1-5-8-17(14(2)3)27-19(23)12-7-11-18(22)26-13-16-10-6-9-15(4)

InchiKey: OFSIPRYWLKNWHI-UHFFFAOYSA-N

Formula: C20H29NO6

SMILES: CCCC(OC(=O)CCCC(=O)OCc1cccc(C)c1[N+](=O)[O-])C(C)C

Mol. weight [g/mol]: 379.45

Physical Properties

Property code	Value	Unit	Source
gf	-226.50	kJ/mol	Joback Method
hf	-753.46	kJ/mol	Joback Method
hfus	50.71	kJ/mol	Joback Method
hvap	97.84	kJ/mol	Joback Method
log10ws	-6.10		Crippen Method
logp	4.485		Crippen Method
mcvol	301.200	ml/mol	McGowan Method
pc	1354.63	kPa	Joback Method
rinpol	2630.00		NIST Webbook
tb	997.18	K	Joback Method
tc	1226.07	K	Joback Method
tf	624.55	K	Joback Method
vc	1.165	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	987.92	J/mol×K	997.18	Joback Method
cpg	1000.35	J/mol×K	1035.33	Joback Method
cpg	1011.33	J/mol×K	1073.48	Joback Method
cpg	1020.91	J/mol×K	1111.63	Joback Method
cpg	1029.10	J/mol×K	1149.77	Joback Method
cpg	1035.94	J/mol×K	1187.92	Joback Method
cpg	1041.47	J/mol×K	1226.07	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U376735&Units=SI
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

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