Glutaric acid, 2-methylhex-3-yl 3-nitro-4-methoxybenzyl ester

Inchi: InChI=1S/C20H29NO7/c1-5-7-17(14(2)3)28-20(23)9-6-8-19(22)27-13-15-10-11-18(26-4)
InchiKey: SBRDMBLPEXVPEJ-UHFFFAOYSA-N
Formula: C20H29NO7
SMILES: CCCC(OC(=O)CCCC(=O)OCc1ccc(OC)c([N+](=O)[O-])c1)C(C)C
Mol. weight [g/mol]: 395.45

Physical Properties

Property code	Value	Unit	Source
gf	-331.50	kJ/mol	Joback Method
hf	-885.68	kJ/mol	Joback Method
hfus	51.90	kJ/mol	Joback Method
hvap	100.25	kJ/mol	Joback Method
log10ws	-5.74		Crippen Method
logp	4.185		Crippen Method
mcvol	307.070	ml/mol	McGowan Method
pc	1337.84	kPa	Joback Method
rinpol	2900.00		NIST Webbook
tb	1019.60	K	Joback Method
tc	1251.02	K	Joback Method
tf	646.78	K	Joback Method
vc	1.183	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1013.77	J/mol×K	1019.60	Joback Method
cpg	1025.08	J/mol×K	1058.17	Joback Method
cpg	1034.75	J/mol×K	1096.74	Joback Method
cpg	1042.78	J/mol×K	1135.31	Joback Method
cpg	1049.20	J/mol×K	1173.88	Joback Method
cpg	1054.02	J/mol×K	1212.45	Joback Method
cpg	1057.24	J/mol×K	1251.02	Joback Method

Sources

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=U377043&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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