Glutaric acid, heptyl 3-nitro-4-methoxybenzyl ester

Inchi: InChI=1S/C20H29NO7/c1-3-4-5-6-7-13-27-19(22)9-8-10-20(23)28-15-16-11-12-18(26-2)
InchiKey: DLFJFNSVJIJXPA-UHFFFAOYSA-N
Formula: C20H29NO7
SMILES: CCCCCCCOC(=O)CCCC(=O)OCc1ccc(OC)c([N+](=O)[O-])c1
Mol. weight [g/mol]: 395.45

Physical Properties

Property code	Value	Unit	Source
gf	-326.62	kJ/mol	Joback Method
hf	-875.12	kJ/mol	Joback Method
hfus	58.94	kJ/mol	Joback Method
hvap	101.03	kJ/mol	Joback Method
log10ws	-5.87		Crippen Method
logp	4.330		Crippen Method
mcvol	307.070	ml/mol	McGowan Method
pc	1322.31	kPa	Joback Method
rinpol	3044.00		NIST Webbook
tb	1020.48	K	Joback Method
tc	1250.53	K	Joback Method
tf	676.78	K	Joback Method
vc	1.196	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1013.05	J/mol×K	1020.48	Joback Method
cpg	1024.45	J/mol×K	1058.82	Joback Method
cpg	1034.24	J/mol×K	1097.16	Joback Method
cpg	1042.45	J/mol×K	1135.50	Joback Method
cpg	1049.10	J/mol×K	1173.85	Joback Method
cpg	1054.19	J/mol×K	1212.19	Joback Method
cpg	1057.73	J/mol×K	1250.53	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=U377045&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