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

Inchi: InChI=1S/C25H39NO7/c1-3-4-5-6-7-8-9-10-11-12-18-32-24(27)14-13-15-25(28)33-20-21

InchiKey: UQHLCKZWCBYGTR-UHFFFAOYSA-N

Formula: C25H39NO7

SMILES: CCCCCCCCCCCCOC(=O)CCCC(=O)OCc1ccc(OC)c([N+](=O)[O-])c1

Mol. weight [g/mol]: 465.58

Physical Properties

Property code	Value	Unit	Source
gf	-284.52	kJ/mol	Joback Method
hf	-978.32	kJ/mol	Joback Method
hfus	71.89	kJ/mol	Joback Method
hvap	112.16	kJ/mol	Joback Method
log10ws	-7.96		Crippen Method
logp	6.281		Crippen Method
mcvol	377.520	ml/mol	McGowan Method
pc	958.51	kPa	Joback Method
rinpol	3563.00		NIST Webbook
rinpol	3563.00		NIST Webbook
tb	1134.88	K	Joback Method
tc	1397.04	K	Joback Method
tf	733.13	K	Joback Method
vc	1.476	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1313.50	J/mol×K	1134.88	Joback Method
cpg	1324.68	J/mol×K	1178.57	Joback Method
cpg	1333.60	J/mol×K	1222.27	Joback Method
cpg	1340.31	J/mol×K	1265.96	Joback Method
cpg	1344.88	J/mol×K	1309.66	Joback Method
cpg	1347.33	J/mol×K	1353.35	Joback Method
cpg	1347.74	J/mol×K	1397.04	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U377050&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