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

Inchi: InChI=1S/C23H35NO7/c1-3-4-5-6-7-8-9-10-16-30-22(25)12-11-13-23(26)31-18-19-14-15

InchiKey: FACUUPNQCYIBNU-UHFFFAOYSA-N

Formula: C23H35NO7

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

Mol. weight [g/mol]: 437.53

Physical Properties

Property code	Value	Unit	Source
gf	-301.36	kJ/mol	Joback Method
hf	-937.04	kJ/mol	Joback Method
hfus	66.71	kJ/mol	Joback Method
hvap	107.70	kJ/mol	Joback Method
log10ws	-7.13		Crippen Method
logp	5.501		Crippen Method
mcvol	349.340	ml/mol	McGowan Method
pc	1083.49	kPa	Joback Method
rinpol	3355.00		NIST Webbook
tb	1089.12	K	Joback Method
tc	1334.76	K	Joback Method
tf	710.59	K	Joback Method
vc	1.363	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1192.53	J/mol×K	1089.12	Joback Method
cpg	1203.83	J/mol×K	1130.06	Joback Method
cpg	1213.21	J/mol×K	1171.00	Joback Method
cpg	1220.68	J/mol×K	1211.94	Joback Method
cpg	1226.28	J/mol×K	1252.88	Joback Method
cpg	1230.04	J/mol×K	1293.82	Joback Method
cpg	1232.00	J/mol×K	1334.76	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=U377048&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