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

Inchi: InChI=1S/C26H41NO7/c1-3-4-5-6-7-8-9-10-11-12-13-19-33-25(28)15-14-16-26(29)34-21
InchiKey: MERKDBBHBTYQTR-UHFFFAOYSA-N
Formula: C26H41NO7
SMILES: CCCCCCCCCCCCCOC(=O)CCCC(=O)OCc1ccc(OC)c([N+](=O)[O-])c1
Mol. weight [g/mol]: 479.61

Physical Properties

Property code	Value	Unit	Source
gf	-276.10	kJ/mol	Joback Method
hf	-998.96	kJ/mol	Joback Method
hfus	74.48	kJ/mol	Joback Method
hvap	114.38	kJ/mol	Joback Method
log10ws	-8.38		Crippen Method
logp	6.671		Crippen Method
mcvol	391.610	ml/mol	McGowan Method
pc	903.97	kPa	Joback Method
rinpol	3712.00		NIST Webbook
rinpol	3712.00		NIST Webbook
tb	1157.76	K	Joback Method
tc	1430.28	K	Joback Method
tf	744.40	K	Joback Method
vc	1.532	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1374.27	J/mol×K	1157.76	Joback Method
cpg	1385.34	J/mol×K	1203.18	Joback Method
cpg	1393.97	J/mol×K	1248.60	Joback Method
cpg	1400.20	J/mol×K	1294.02	Joback Method
cpg	1404.11	J/mol×K	1339.44	Joback Method
cpg	1405.76	J/mol×K	1384.86	Joback Method
cpg	1405.20	J/mol×K	1430.28	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=U377051&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