Glutaric acid, 2-nitro-3-chlorobenzyl tridecyl ester

Inchi: InChI=1S/C25H38ClNO6/c1-2-3-4-5-6-7-8-9-10-11-12-19-32-23(28)17-14-18-24(29)33-2
InchiKey: POGLTADSTRKPMI-UHFFFAOYSA-N
Formula: C25H38ClNO6
SMILES: CCCCCCCCCCCCCOC(=O)CCCC(=O)OCc1cccc(Cl)c1[N+](=O)[O-]
Mol. weight [g/mol]: 484.02

Physical Properties

Property code	Value	Unit	Source
gf	-191.45	kJ/mol	Joback Method
hf	-861.84	kJ/mol	Joback Method
hfus	74.90	kJ/mol	Joback Method
hvap	114.13	kJ/mol	Joback Method
log10ws	-8.95		Crippen Method
logp	7.316		Crippen Method
mcvol	383.890	ml/mol	McGowan Method
pc	946.75	kPa	Joback Method
rinpol	3516.00		NIST Webbook
rinpol	3516.00		NIST Webbook
tb	1149.89	K	Joback Method
tc	1415.18	K	Joback Method
tf	740.82	K	Joback Method
vc	1.506	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1308.72	J/mol×K	1149.89	Joback Method
cpg	1320.33	J/mol×K	1194.10	Joback Method
cpg	1330.02	J/mol×K	1238.32	Joback Method
cpg	1337.89	J/mol×K	1282.53	Joback Method
cpg	1344.02	J/mol×K	1326.75	Joback Method
cpg	1348.50	J/mol×K	1370.96	Joback Method
cpg	1351.40	J/mol×K	1415.18	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=U377036&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