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

Inchi: InChI=1S/C22H32ClNO6/c1-2-3-4-5-6-7-8-9-16-29-20(25)14-11-15-21(26)30-17-18-12-1

InchiKey: RXAZBVGKVQJPOG-UHFFFAOYSA-N

Formula: C22H32ClNO6

SMILES: CCCCCCCCCCOC(=O)CCCC(=O)OCc1cccc(Cl)c1[N+](=O)[O-]

Mol. weight [g/mol]: 441.95

Physical Properties

Property code	Value	Unit	Source
gf	-216.71	kJ/mol	Joback Method
hf	-799.92	kJ/mol	Joback Method
hfus	67.13	kJ/mol	Joback Method
hvap	107.45	kJ/mol	Joback Method
log10ws	-7.69		Crippen Method
logp	6.146		Crippen Method
mcvol	341.620	ml/mol	McGowan Method
pc	1139.80	kPa	Joback Method
rinpol	3188.00		NIST Webbook
rinpol	3188.00		NIST Webbook
tb	1081.25	K	Joback Method
tc	1323.87	K	Joback Method
tf	707.01	K	Joback Method
vc	1.339	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1126.96	J/mol×K	1081.25	Joback Method
cpg	1138.28	J/mol×K	1121.69	Joback Method
cpg	1148.02	J/mol×K	1162.12	Joback Method
cpg	1156.25	J/mol×K	1202.56	Joback Method
cpg	1163.00	J/mol×K	1243.00	Joback Method
cpg	1168.33	J/mol×K	1283.44	Joback Method
cpg	1172.30	J/mol×K	1323.87	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=U377033&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