Glutaric acid, 2-methylhex-3-yl 2-nitro-3-chlorobenzyl ester

Inchi: InChI=1S/C19H26ClNO6/c1-4-7-16(13(2)3)27-18(23)11-6-10-17(22)26-12-14-8-5-9-15(2

InchiKey: YQDWTPNFROSEML-UHFFFAOYSA-N

Formula: C19H26ClNO6

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

Mol. weight [g/mol]: 399.87

Physical Properties

Property code	Value	Unit	Source
gf	-246.85	kJ/mol	Joback Method
hf	-748.56	kJ/mol	Joback Method
hfus	52.31	kJ/mol	Joback Method
hvap	100.00	kJ/mol	Joback Method
log10ws	-6.31		Crippen Method
logp	4.830		Crippen Method
mcvol	299.350	ml/mol	McGowan Method
pc	1415.44	kPa	Joback Method
rinpol	2722.00		NIST Webbook
rinpol	2722.00		NIST Webbook
tb	1011.73	K	Joback Method
tc	1244.63	K	Joback Method
tf	643.20	K	Joback Method
vc	1.159	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	949.17	J/mol×K	1011.73	Joback Method
cpg	960.18	J/mol×K	1050.55	Joback Method
cpg	969.79	J/mol×K	1089.36	Joback Method
cpg	978.01	J/mol×K	1128.18	Joback Method
cpg	984.90	J/mol×K	1167.00	Joback Method
cpg	990.47	J/mol×K	1205.81	Joback Method
cpg	994.76	J/mol×K	1244.63	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U377028&Units=SI

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