Glutaric acid, 3-chlorophenyl 3-nitrobenzyl ester

Inchi: InChI=1S/C18H16ClNO6/c19-14-5-2-7-16(11-14)26-18(22)9-3-8-17(21)25-12-13-4-1-6-1

InchiKey: KFXCOUACLFYBNQ-UHFFFAOYSA-N

Formula: C18H16ClNO6

SMILES: O=C(CCCC(=O)Oc1cccc(Cl)c1)OCc1cccc([N+](=O)[O-])c1

Mol. weight [g/mol]: 377.78

Physical Properties

Property code	Value	Unit	Source
gf	-137.98	kJ/mol	Joback Method
hf	-480.83	kJ/mol	Joback Method
hfus	50.81	kJ/mol	Joback Method
hvap	100.83	kJ/mol	Joback Method
log10ws	-5.77		Crippen Method
logp	4.067		Crippen Method
mcvol	261.500	ml/mol	McGowan Method
pc	1980.59	kPa	Joback Method
rinpol	3085.00		NIST Webbook
rinpol	3085.00		NIST Webbook
tb	1016.41	K	Joback Method
tc	1266.82	K	Joback Method
tf	688.35	K	Joback Method
vc	1.006	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	778.05	J/mol×K	1016.41	Joback Method
cpg	786.42	J/mol×K	1058.14	Joback Method
cpg	793.44	J/mol×K	1099.88	Joback Method
cpg	799.15	J/mol×K	1141.61	Joback Method
cpg	803.59	J/mol×K	1183.35	Joback Method
cpg	806.82	J/mol×K	1225.08	Joback Method
cpg	808.88	J/mol×K	1266.82	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=U393360&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