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

Inchi: InChI=1S/C15H18ClNO6/c1-2-9-22-13(18)7-4-8-14(19)23-10-11-5-3-6-12(16)15(11)17(2
InchiKey: ZWQYQMQLIZZCQB-UHFFFAOYSA-N
Formula: C15H18ClNO6
SMILES: CCCOC(=O)CCCC(=O)OCc1cccc(Cl)c1[N+](=O)[O-]
Mol. weight [g/mol]: 343.76

Physical Properties

Property code	Value	Unit	Source
gf	-275.65	kJ/mol	Joback Method
hf	-655.44	kJ/mol	Joback Method
hfus	49.00	kJ/mol	Joback Method
hvap	91.87	kJ/mol	Joback Method
log10ws	-4.76		Crippen Method
logp	3.415		Crippen Method
mcvol	242.990	ml/mol	McGowan Method
pc	1906.90	kPa	Joback Method
rinpol	2458.00		NIST Webbook
tb	921.09	K	Joback Method
tc	1149.20	K	Joback Method
tf	628.12	K	Joback Method
vc	0.947	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	717.52	J/mol×K	921.09	Joback Method
cpg	728.07	J/mol×K	959.11	Joback Method
cpg	737.46	J/mol×K	997.13	Joback Method
cpg	745.71	J/mol×K	1035.15	Joback Method
cpg	752.82	J/mol×K	1073.16	Joback Method
cpg	758.81	J/mol×K	1111.18	Joback Method
cpg	763.71	J/mol×K	1149.20	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U377024&Units=SI
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

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