Glutaric acid, 8-chlorooctyl 2-nitrophenyl ester

Inchi: InChI=1S/C19H26ClNO6/c20-14-7-3-1-2-4-8-15-26-18(22)12-9-13-19(23)27-17-11-6-5-1
InchiKey: YAKFMOGSBNBERQ-UHFFFAOYSA-N
Formula: C19H26ClNO6
SMILES: O=C(CCCC(=O)Oc1ccccc1[N+](=O)[O-])OCCCCCCCCCl
Mol. weight [g/mol]: 399.87

Physical Properties

Property code	Value	Unit	Source
gf	-232.34	kJ/mol	Joback Method
hf	-726.53	kJ/mol	Joback Method
hfus	59.75	kJ/mol	Joback Method
hvap	100.11	kJ/mol	Joback Method
log10ws	-6.06		Crippen Method
logp	4.793		Crippen Method
mcvol	299.350	ml/mol	McGowan Method
pc	1414.37	kPa	Joback Method
rinpol	3094.00		NIST Webbook
rinpol	3094.00		NIST Webbook
tb	1007.63	K	Joback Method
tc	1237.32	K	Joback Method
tf	660.68	K	Joback Method
vc	1.171	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	949.93	J/mol×K	1007.63	Joback Method
cpg	961.13	J/mol×K	1045.91	Joback Method
cpg	971.03	J/mol×K	1084.19	Joback Method
cpg	979.65	J/mol×K	1122.47	Joback Method
cpg	987.05	J/mol×K	1160.76	Joback Method
cpg	993.24	J/mol×K	1199.04	Joback Method
cpg	998.29	J/mol×K	1237.32	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393323&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