Glutaric acid, 2,3-dichlorophenyl 3-nitrobenzyl ester

Inchi: InChI=1S/C18H15Cl2NO6/c19-14-6-2-7-15(18(14)20)27-17(23)9-3-8-16(22)26-11-12-4-1

InchiKey: ACCSGQRHDZUARM-UHFFFAOYSA-N

Formula: C18H15Cl2NO6

SMILES: O=C(CCCC(=O)Oc1cccc(Cl)c1Cl)OCc1cccc([N+](=O)[O-])c1

Mol. weight [g/mol]: 412.22

Physical Properties

Property code	Value	Unit	Source
gf	-159.54	kJ/mol	Joback Method
hf	-508.04	kJ/mol	Joback Method
hfus	54.62	kJ/mol	Joback Method
hvap	105.87	kJ/mol	Joback Method
log10ws	-6.45		Crippen Method
logp	4.721		Crippen Method
mcvol	273.740	ml/mol	McGowan Method
pc	1892.00	kPa	Joback Method
rinpol	3253.00		NIST Webbook
rinpol	3253.00		NIST Webbook
tb	1058.82	K	Joback Method
tc	1313.59	K	Joback Method
tf	730.79	K	Joback Method
vc	1.056	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	791.35	J/mol×K	1058.82	Joback Method
cpg	798.13	J/mol×K	1101.28	Joback Method
cpg	803.54	J/mol×K	1143.74	Joback Method
cpg	807.62	J/mol×K	1186.20	Joback Method
cpg	810.40	J/mol×K	1228.66	Joback Method
cpg	811.94	J/mol×K	1271.13	Joback Method
cpg	812.26	J/mol×K	1313.59	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=U393362&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