Glutaric acid, di(2-nitro-3-chlorobenzyl) ester

Inchi: InChI=1S/C19H16Cl2N2O8/c20-14-6-1-4-12(18(14)22(26)27)10-30-16(24)8-3-9-17(25)31
InchiKey: SVUQYHGIUOWDGH-UHFFFAOYSA-N
Formula: C19H16Cl2N2O8
SMILES: O=C(CCCC(=O)OCc1cccc(Cl)c1[N+](=O)[O-])OCc1cccc(Cl)c1[N+](=O)[O-]
Mol. weight [g/mol]: 471.25

Physical Properties

Property code	Value	Unit	Source
gf	-125.20	kJ/mol	Joback Method
hf	-550.91	kJ/mol	Joback Method
hfus	68.18	kJ/mol	Joback Method
hvap	125.35	kJ/mol	Joback Method
log10ws	-7.37		Crippen Method
logp	4.767		Crippen Method
mcvol	305.250	ml/mol	McGowan Method
pc	1739.01	kPa	Joback Method
rinpol	3752.00		NIST Webbook
rinpol	3752.00		NIST Webbook
tb	1238.52	K	Joback Method
tc	1518.57	K	Joback Method
tf	898.19	K	Joback Method
vc	1.194	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	908.82	J/mol×K	1238.52	Joback Method
cpg	910.20	J/mol×K	1285.20	Joback Method
cpg	909.95	J/mol×K	1331.87	Joback Method
cpg	908.15	J/mol×K	1378.55	Joback Method
cpg	904.84	J/mol×K	1425.22	Joback Method
cpg	900.10	J/mol×K	1471.90	Joback Method
cpg	893.97	J/mol×K	1518.57	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=U377037&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