Succinic acid, di(4-chloro-2-nitrobenzyl) ester

Inchi: InChI=1S/C18H14Cl2N2O8/c19-13-3-1-11(15(7-13)21(25)26)9-29-17(23)5-6-18(24)30-10
InchiKey: POCUHZQODMUMII-UHFFFAOYSA-N
Formula: C18H14Cl2N2O8
SMILES: O=C(CCC(=O)OCc1ccc(Cl)cc1[N+](=O)[O-])OCc1ccc(Cl)cc1[N+](=O)[O-]
Mol. weight [g/mol]: 457.22

Physical Properties

Property code	Value	Unit	Source
gf	-133.62	kJ/mol	Joback Method
hf	-530.27	kJ/mol	Joback Method
hfus	65.59	kJ/mol	Joback Method
hvap	123.13	kJ/mol	Joback Method
log10ws	-6.95		Crippen Method
logp	4.377		Crippen Method
mcvol	291.160	ml/mol	McGowan Method
pc	1887.08	kPa	Joback Method
rinpol	3346.00		NIST Webbook
rinpol	3346.00		NIST Webbook
tb	1215.64	K	Joback Method
tc	1493.60	K	Joback Method
tf	886.92	K	Joback Method
vc	1.137	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	851.98	J/mol×K	1215.64	Joback Method
cpg	853.46	J/mol×K	1261.97	Joback Method
cpg	853.36	J/mol×K	1308.29	Joback Method
cpg	851.73	J/mol×K	1354.62	Joback Method
cpg	848.61	J/mol×K	1400.94	Joback Method
cpg	844.07	J/mol×K	1447.27	Joback Method
cpg	838.14	J/mol×K	1493.60	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=U380946&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