Succinic acid, 4-chloro-2-nitrobenzyl ethyl ester

Inchi: InChI=1S/C13H14ClNO6/c1-2-20-12(16)5-6-13(17)21-8-9-3-4-10(14)7-11(9)15(18)19/h3-

InchiKey: SAJOCWCIKHBNFO-UHFFFAOYSA-N

Formula: C13H14ClNO6

SMILES: CCOC(=O)CCC(=O)OCc1ccc(Cl)cc1[N+](=O)[O-]

Mol. weight [g/mol]: 315.71

Physical Properties

Property code	Value	Unit	Source
gf	-292.49	kJ/mol	Joback Method
hf	-614.16	kJ/mol	Joback Method
hfus	43.82	kJ/mol	Joback Method
hvap	87.42	kJ/mol	Joback Method
log10ws	-3.92		Crippen Method
logp	2.635		Crippen Method
mcvol	214.810	ml/mol	McGowan Method
pc	2271.90	kPa	Joback Method
rinpol	2253.00		NIST Webbook
rinpol	2253.00		NIST Webbook
tb	875.33	K	Joback Method
tc	1107.00	K	Joback Method
tf	605.58	K	Joback Method
vc	0.835	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	606.16	J/mol×K	875.33	Joback Method
cpg	616.28	J/mol×K	913.94	Joback Method
cpg	625.32	J/mol×K	952.55	Joback Method
cpg	633.27	J/mol×K	991.16	Joback Method
cpg	640.16	J/mol×K	1029.78	Joback Method
cpg	645.98	J/mol×K	1068.39	Joback Method
cpg	650.74	J/mol×K	1107.00	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U380935&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