Succinic acid, 3-chloro-2-nitrobenzyl 2-methylhex-3-yl ester

Inchi: InChI=1S/C18H24ClNO6/c1-4-6-15(12(2)3)26-17(22)10-9-16(21)25-11-13-7-5-8-14(19)1

InchiKey: XNSVPJCQVGURET-UHFFFAOYSA-N

Formula: C18H24ClNO6

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

Mol. weight [g/mol]: 385.84

Physical Properties

Property code	Value	Unit	Source
gf	-255.27	kJ/mol	Joback Method
hf	-727.92	kJ/mol	Joback Method
hfus	49.72	kJ/mol	Joback Method
hvap	97.77	kJ/mol	Joback Method
log10ws	-5.89		Crippen Method
logp	4.439		Crippen Method
mcvol	285.260	ml/mol	McGowan Method
pc	1523.50	kPa	Joback Method
rinpol	2585.00		NIST Webbook
rinpol	2585.00		NIST Webbook
tb	988.85	K	Joback Method
tc	1220.58	K	Joback Method
tf	631.93	K	Joback Method
vc	1.103	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	890.67	J/mol×K	988.85	Joback Method
cpg	901.63	J/mol×K	1027.47	Joback Method
cpg	911.24	J/mol×K	1066.09	Joback Method
cpg	919.51	J/mol×K	1104.71	Joback Method
cpg	926.48	J/mol×K	1143.34	Joback Method
cpg	932.17	J/mol×K	1181.96	Joback Method
cpg	936.61	J/mol×K	1220.58	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=U380960&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