Succinic acid, 3-chloro-2-nitrobenzyl isobutyl ester

Inchi: InChI=1S/C15H18ClNO6/c1-10(2)8-22-13(18)6-7-14(19)23-9-11-4-3-5-12(16)15(11)17(2

InchiKey: IPIMMASUBRHOJF-UHFFFAOYSA-N

Formula: C15H18ClNO6

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

Mol. weight [g/mol]: 343.76

Physical Properties

Property code	Value	Unit	Source
gf	-278.09	kJ/mol	Joback Method
hf	-660.72	kJ/mol	Joback Method
hfus	45.48	kJ/mol	Joback Method
hvap	91.48	kJ/mol	Joback Method
log10ws	-4.52		Crippen Method
logp	3.271		Crippen Method
mcvol	242.990	ml/mol	McGowan Method
pc	1920.30	kPa	Joback Method
rinpol	2382.00		NIST Webbook
rinpol	2382.00		NIST Webbook
tb	920.65	K	Joback Method
tc	1151.32	K	Joback Method
tf	613.12	K	Joback Method
vc	0.941	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	718.06	J/mol×K	920.65	Joback Method
cpg	728.68	J/mol×K	959.10	Joback Method
cpg	738.10	J/mol×K	997.54	Joback Method
cpg	746.34	J/mol×K	1035.99	Joback Method
cpg	753.40	J/mol×K	1074.43	Joback Method
cpg	759.31	J/mol×K	1112.88	Joback Method
cpg	764.08	J/mol×K	1151.32	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=U380957&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