Succinic acid, 2-methyl-3-nitrobenzyl pentyl ester

Inchi: InChI=1S/C17H23NO6/c1-3-4-5-11-23-16(19)9-10-17(20)24-12-14-7-6-8-15(13(14)2)18(
InchiKey: JAOTUGMPCUYTIG-UHFFFAOYSA-N
Formula: C17H23NO6
SMILES: CCCCCOC(=O)CCC(=O)OCc1cccc([N+](=O)[O-])c1C
Mol. weight [g/mol]: 337.37

Physical Properties

Property code	Value	Unit	Source
gf	-246.88	kJ/mol	Joback Method
hf	-680.98	kJ/mol	Joback Method
hfus	49.98	kJ/mol	Joback Method
hvap	91.94	kJ/mol	Joback Method
log10ws	-4.97		Crippen Method
logp	3.460		Crippen Method
mcvol	258.930	ml/mol	McGowan Method
pc	1672.79	kPa	Joback Method
rinpol	2526.00		NIST Webbook
rinpol	2526.00		NIST Webbook
tb	929.42	K	Joback Method
tc	1152.32	K	Joback Method
tf	620.74	K	Joback Method
vc	1.010	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	811.03	J/mol×K	929.42	Joback Method
cpg	823.17	J/mol×K	966.57	Joback Method
cpg	834.07	J/mol×K	1003.72	Joback Method
cpg	843.77	J/mol×K	1040.87	Joback Method
cpg	852.26	J/mol×K	1078.02	Joback Method
cpg	859.58	J/mol×K	1115.17	Joback Method
cpg	865.74	J/mol×K	1152.32	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=U380843&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