Succinic acid, 2-ethylhexyl 3-nitrobenzyl ester

Inchi: InChI=1S/C19H27NO6/c1-3-5-7-15(4-2)13-25-18(21)10-11-19(22)26-14-16-8-6-9-17(12-
InchiKey: DGVHIGKHQKJCJK-UHFFFAOYSA-N
Formula: C19H27NO6
SMILES: CCCCC(CC)COC(=O)CCC(=O)OCc1cccc([N+](=O)[O-])c1
Mol. weight [g/mol]: 365.42

Physical Properties

Property code	Value	Unit	Source
gf	-222.85	kJ/mol	Joback Method
hf	-716.07	kJ/mol	Joback Method
hfus	52.03	kJ/mol	Joback Method
hvap	95.34	kJ/mol	Joback Method
log10ws	-5.51		Crippen Method
logp	4.178		Crippen Method
mcvol	287.110	ml/mol	McGowan Method
pc	1463.49	kPa	Joback Method
rinpol	2760.00		NIST Webbook
rinpol	2760.00		NIST Webbook
tb	969.76	K	Joback Method
tc	1194.84	K	Joback Method
tf	615.76	K	Joback Method
vc	1.115	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	929.61	J/mol×K	969.76	Joback Method
cpg	942.12	J/mol×K	1007.27	Joback Method
cpg	953.29	J/mol×K	1044.79	Joback Method
cpg	963.17	J/mol×K	1082.30	Joback Method
cpg	971.79	J/mol×K	1119.81	Joback Method
cpg	979.18	J/mol×K	1157.33	Joback Method
cpg	985.37	J/mol×K	1194.84	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=U390181&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