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

Inchi: InChI=1S/C18H25NO6/c1-4-6-16(13(2)3)25-18(21)10-9-17(20)24-12-14-7-5-8-15(11-14)
InchiKey: VQTBUSBLVHUMBZ-UHFFFAOYSA-N
Formula: C18H25NO6
SMILES: CCCC(OC(=O)CCC(=O)OCc1cccc([N+](=O)[O-])c1)C(C)C
Mol. weight [g/mol]: 351.39

Physical Properties

Property code	Value	Unit	Source
gf	-233.71	kJ/mol	Joback Method
hf	-700.71	kJ/mol	Joback Method
hfus	45.92	kJ/mol	Joback Method
hvap	92.73	kJ/mol	Joback Method
log10ws	-5.20		Crippen Method
logp	3.786		Crippen Method
mcvol	273.020	ml/mol	McGowan Method
pc	1587.28	kPa	Joback Method
rinpol	2532.00		NIST Webbook
rinpol	2532.00		NIST Webbook
tb	946.44	K	Joback Method
tc	1172.55	K	Joback Method
tf	589.49	K	Joback Method
vc	1.054	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	871.42	J/mol×K	946.44	Joback Method
cpg	883.89	J/mol×K	984.13	Joback Method
cpg	895.04	J/mol×K	1021.81	Joback Method
cpg	904.89	J/mol×K	1059.50	Joback Method
cpg	913.48	J/mol×K	1097.18	Joback Method
cpg	920.85	J/mol×K	1134.87	Joback Method
cpg	927.01	J/mol×K	1172.55	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U381690&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