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

Inchi: InChI=1S/C18H25NO6/c1-3-4-5-6-12-24-16(20)10-11-17(21)25-13-15-9-7-8-14(2)18(15)19(22)23

InchiKey: GMFHJDXJHMSXFT-UHFFFAOYSA-N

Formula: C18H25NO6

SMILES: CCCCCCOC(=O)CCC(=O)OCc1cccc(C)c1[N+](=O)[O-]

Mol. weight [g/mol]: 351.39

Physical Properties

Property code	Value	Unit	Source
gf	-238.46	kJ/mol	Joback Method
hf	-701.62	kJ/mol	Joback Method
hfus	52.57	kJ/mol	Joback Method
hvap	94.17	kJ/mol	Joback Method
log10ws	-5.39		Crippen Method
logp	3.850		Crippen Method
mcvol	273.020	ml/mol	McGowan Method
pc	1548.78	kPa	Joback Method
rinpol	2550.00		NIST Webbook
rinpol	2550.00		NIST Webbook
tb	952.30	K	Joback Method
tc	1175.63	K	Joback Method
tf	632.01	K	Joback Method
vc	1.065	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	869.16	J/mol×K	952.30	Joback Method
cpg	881.41	J/mol×K	989.52	Joback Method
cpg	892.39	J/mol×K	1026.74	Joback Method
cpg	902.11	J/mol×K	1063.97	Joback Method
cpg	910.59	J/mol×K	1101.19	Joback Method
cpg	917.87	J/mol×K	1138.41	Joback Method
cpg	923.95	J/mol×K	1175.63	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U380969&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