Succinic acid, di(3-nitrobenzyl) ester

Inchi: InChI=1S/C18H16N2O8/c21-17(27-11-13-3-1-5-15(9-13)19(23)24)7-8-18(22)28-12-14-4-
InchiKey: WRYOAEOXYJLBOY-UHFFFAOYSA-N
Formula: C18H16N2O8
SMILES: O=C(CCC(=O)OCc1cccc([N+](=O)[O-])c1)OCc1cccc([N+](=O)[O-])c1
Mol. weight [g/mol]: 388.33

Physical Properties

Property code	Value	Unit	Source
gf	-90.50	kJ/mol	Joback Method
hf	-475.85	kJ/mol	Joback Method
hfus	57.98	kJ/mol	Joback Method
hvap	113.03	kJ/mol	Joback Method
log10ws	-5.58		Crippen Method
logp	3.070		Crippen Method
mcvol	266.680	ml/mol	McGowan Method
pc	2069.88	kPa	Joback Method
rinpol	3416.00		NIST Webbook
rinpol	3416.00		NIST Webbook
tb	1130.82	K	Joback Method
tc	1397.42	K	Joback Method
tf	802.04	K	Joback Method
vc	1.040	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	836.51	J/mol×K	1130.82	Joback Method
cpg	841.63	J/mol×K	1175.25	Joback Method
cpg	845.28	J/mol×K	1219.69	Joback Method
cpg	847.53	J/mol×K	1264.12	Joback Method
cpg	848.42	J/mol×K	1308.55	Joback Method
cpg	848.04	J/mol×K	1352.99	Joback Method
cpg	846.43	J/mol×K	1397.42	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U381693&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