Succinic acid, di(2-(3-nitrophenyl)ethyl) ester

Inchi: InChI=1S/C20H20N2O8/c23-19(29-11-9-15-3-1-5-17(13-15)21(25)26)7-8-20(24)30-12-10
InchiKey: QZNFUGBNVRODOS-UHFFFAOYSA-N
Formula: C20H20N2O8
SMILES: O=C(CCC(=O)OCCc1cccc([N+](=O)[O-])c1)OCCc1cccc([N+](=O)[O-])c1
Mol. weight [g/mol]: 416.38

Physical Properties

Property code	Value	Unit	Source
gf	-73.66	kJ/mol	Joback Method
hf	-517.13	kJ/mol	Joback Method
hfus	63.16	kJ/mol	Joback Method
hvap	117.48	kJ/mol	Joback Method
log10ws	-5.43		Crippen Method
logp	3.155		Crippen Method
mcvol	294.860	ml/mol	McGowan Method
pc	1750.67	kPa	Joback Method
rinpol	3437.00		NIST Webbook
rinpol	3437.00		NIST Webbook
tb	1176.58	K	Joback Method
tc	1444.76	K	Joback Method
tf	824.58	K	Joback Method
vc	1.151	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	951.64	J/mol×K	1176.58	Joback Method
cpg	956.69	J/mol×K	1221.28	Joback Method
cpg	960.22	J/mol×K	1265.97	Joback Method
cpg	962.33	J/mol×K	1310.67	Joback Method
cpg	963.07	J/mol×K	1355.37	Joback Method
cpg	962.54	J/mol×K	1400.07	Joback Method
cpg	960.80	J/mol×K	1444.76	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=U381003&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