Succinic acid, 3,5-dinitrobenzyl nonyl ester

Inchi: InChI=1S/C20H28N2O8/c1-2-3-4-5-6-7-8-11-29-19(23)9-10-20(24)30-15-16-12-17(21(25
InchiKey: ZPVYPHCNSAPBGY-UHFFFAOYSA-N
Formula: C20H28N2O8
SMILES: CCCCCCCCCOC(=O)CCC(=O)OCc1cc([N+](=O)[O-])cc([N+](=O)[O-])c1
Mol. weight [g/mol]: 424.44

Physical Properties

Property code	Value	Unit	Source
gf	-186.07	kJ/mol	Joback Method
hf	-753.66	kJ/mol	Joback Method
hfus	69.12	kJ/mol	Joback Method
hvap	115.21	kJ/mol	Joback Method
log10ws	-6.82		Crippen Method
logp	4.620		Crippen Method
mcvol	318.620	ml/mol	McGowan Method
pc	1350.65	kPa	Joback Method
rinpol	3158.00		NIST Webbook
rinpol	3158.00		NIST Webbook
tb	1149.90	K	Joback Method
tc	1407.83	K	Joback Method
tf	798.16	K	Joback Method
vc	1.260	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1075.02	J/mol×K	1149.90	Joback Method
cpg	1082.82	J/mol×K	1192.89	Joback Method
cpg	1088.96	J/mol×K	1235.88	Joback Method
cpg	1093.50	J/mol×K	1278.86	Joback Method
cpg	1096.48	J/mol×K	1321.85	Joback Method
cpg	1097.97	J/mol×K	1364.84	Joback Method
cpg	1098.02	J/mol×K	1407.83	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U381097&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