Succinic acid, 3,5-dinitrobenzyl ethyl ester

Inchi: InChI=1S/C13H14N2O8/c1-2-22-12(16)3-4-13(17)23-8-9-5-10(14(18)19)7-11(6-9)15(20)
InchiKey: ARJZQKPMMNDTOX-UHFFFAOYSA-N
Formula: C13H14N2O8
SMILES: CCOC(=O)CCC(=O)OCc1cc([N+](=O)[O-])cc([N+](=O)[O-])c1
Mol. weight [g/mol]: 326.26

Physical Properties

Property code	Value	Unit	Source
gf	-245.01	kJ/mol	Joback Method
hf	-609.18	kJ/mol	Joback Method
hfus	50.98	kJ/mol	Joback Method
hvap	99.63	kJ/mol	Joback Method
log10ws	-3.89		Crippen Method
logp	1.889		Crippen Method
mcvol	219.990	ml/mol	McGowan Method
pc	2381.86	kPa	Joback Method
rinpol	2475.00		NIST Webbook
rinpol	2475.00		NIST Webbook
tb	989.74	K	Joback Method
tc	1236.64	K	Joback Method
tf	719.27	K	Joback Method
vc	0.868	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	670.87	J/mol×K	989.74	Joback Method
cpg	678.55	J/mol×K	1030.89	Joback Method
cpg	684.95	J/mol×K	1072.04	Joback Method
cpg	690.07	J/mol×K	1113.19	Joback Method
cpg	693.92	J/mol×K	1154.34	Joback Method
cpg	696.51	J/mol×K	1195.49	Joback Method
cpg	697.87	J/mol×K	1236.64	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U381091&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

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

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