Succinic acid, 3,5-dinitro-2-methylbenzyl ethyl ester

Inchi: InChI=1S/C14H16N2O8/c1-3-23-13(17)4-5-14(18)24-8-10-6-11(15(19)20)7-12(9(10)2)16

InchiKey: CNYDCBGTLQGABO-UHFFFAOYSA-N

Formula: C14H16N2O8

SMILES: CCOC(=O)CCC(=O)OCc1cc([N+](=O)[O-])cc([N+](=O)[O-])c1C

Mol. weight [g/mol]: 340.29

Physical Properties

Property code	Value	Unit	Source
gf	-246.22	kJ/mol	Joback Method
hf	-641.29	kJ/mol	Joback Method
hfus	53.19	kJ/mol	Joback Method
hvap	102.51	kJ/mol	Joback Method
log10ws	-4.36		Crippen Method
logp	2.198		Crippen Method
mcvol	234.080	ml/mol	McGowan Method
pc	2143.35	kPa	Joback Method
rinpol	2563.00		NIST Webbook
rinpol	2563.00		NIST Webbook
tb	1017.60	K	Joback Method
tc	1263.91	K	Joback Method
tf	743.06	K	Joback Method
vc	0.923	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	725.14	J/mol×K	1017.60	Joback Method
cpg	732.75	J/mol×K	1058.65	Joback Method
cpg	738.98	J/mol×K	1099.70	Joback Method
cpg	743.85	J/mol×K	1140.75	Joback Method
cpg	747.35	J/mol×K	1181.81	Joback Method
cpg	749.51	J/mol×K	1222.86	Joback Method
cpg	750.32	J/mol×K	1263.91	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U381004&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