Succinic acid, 3,5-dinitrobenzyl pentyl ester

Inchi: InChI=1S/C16H20N2O8/c1-2-3-4-7-25-15(19)5-6-16(20)26-11-12-8-13(17(21)22)10-14(9
InchiKey: LXKTXEQFMIEWFO-UHFFFAOYSA-N
Formula: C16H20N2O8
SMILES: CCCCCOC(=O)CCC(=O)OCc1cc([N+](=O)[O-])cc([N+](=O)[O-])c1
Mol. weight [g/mol]: 368.34

Physical Properties

Property code	Value	Unit	Source
gf	-219.75	kJ/mol	Joback Method
hf	-671.10	kJ/mol	Joback Method
hfus	58.75	kJ/mol	Joback Method
hvap	106.30	kJ/mol	Joback Method
log10ws	-5.14		Crippen Method
logp	3.060		Crippen Method
mcvol	262.260	ml/mol	McGowan Method
pc	1830.98	kPa	Joback Method
rinpol	2764.00		NIST Webbook
rinpol	2764.00		NIST Webbook
tb	1058.38	K	Joback Method
tc	1303.94	K	Joback Method
tf	753.08	K	Joback Method
vc	1.036	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	841.39	J/mol×K	1058.38	Joback Method
cpg	849.26	J/mol×K	1099.31	Joback Method
cpg	855.72	J/mol×K	1140.23	Joback Method
cpg	860.80	J/mol×K	1181.16	Joback Method
cpg	864.52	J/mol×K	1222.09	Joback Method
cpg	866.91	J/mol×K	1263.01	Joback Method
cpg	868.01	J/mol×K	1303.94	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U381094&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