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

Inchi: InChI=1S/C18H24N2O8/c1-3-4-5-6-9-27-17(21)7-8-18(22)28-12-14-10-15(19(23)24)11-1

InchiKey: PDMRAFARUAXFCK-UHFFFAOYSA-N

Formula: C18H24N2O8

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

Mol. weight [g/mol]: 396.39

Physical Properties

Property code	Value	Unit	Source
gf	-212.54	kJ/mol	Joback Method
hf	-723.85	kJ/mol	Joback Method
hfus	63.55	kJ/mol	Joback Method
hvap	111.42	kJ/mol	Joback Method
log10ws	-6.04		Crippen Method
logp	3.758		Crippen Method
mcvol	290.440	ml/mol	McGowan Method
pc	1545.13	kPa	Joback Method
rinpol	2935.00		NIST Webbook
rinpol	2935.00		NIST Webbook
tb	1109.12	K	Joback Method
tc	1359.63	K	Joback Method
tf	788.14	K	Joback Method
vc	1.147	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	955.31	J/mol×K	1109.12	Joback Method
cpg	962.88	J/mol×K	1150.87	Joback Method
cpg	968.85	J/mol×K	1192.62	Joback Method
cpg	973.27	J/mol×K	1234.38	Joback Method
cpg	976.15	J/mol×K	1276.13	Joback Method
cpg	977.53	J/mol×K	1317.88	Joback Method
cpg	977.44	J/mol×K	1359.63	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U381010&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