Succinic acid, 3,5-dinitrobenzyl 2-methylhex-3-yl ester

Inchi: InChI=1S/C18H24N2O8/c1-4-5-16(12(2)3)28-18(22)7-6-17(21)27-11-13-8-14(19(23)24)1

InchiKey: PDSDIXGLHWKOMJ-UHFFFAOYSA-N

Formula: C18H24N2O8

SMILES: CCCC(OC(=O)CCC(=O)OCc1cc([N+](=O)[O-])cc([N+](=O)[O-])c1)C(C)C

Mol. weight [g/mol]: 396.39

Physical Properties

Property code	Value	Unit	Source
gf	-207.79	kJ/mol	Joback Method
hf	-722.94	kJ/mol	Joback Method
hfus	56.89	kJ/mol	Joback Method
hvap	109.98	kJ/mol	Joback Method
log10ws	-5.85		Crippen Method
logp	3.694		Crippen Method
mcvol	290.440	ml/mol	McGowan Method
pc	1583.49	kPa	Joback Method
rinpol	2809.00		NIST Webbook
rinpol	2809.00		NIST Webbook
tb	1103.26	K	Joback Method
tc	1354.58	K	Joback Method
tf	745.62	K	Joback Method
vc	1.135	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	957.85	J/mol×K	1103.26	Joback Method
cpg	965.53	J/mol×K	1145.15	Joback Method
cpg	971.64	J/mol×K	1187.03	Joback Method
cpg	976.21	J/mol×K	1228.92	Joback Method
cpg	979.29	J/mol×K	1270.81	Joback Method
cpg	980.91	J/mol×K	1312.70	Joback Method
cpg	981.12	J/mol×K	1354.58	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U381095&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