Succinic acid, 3,5-dinitro-4-methylbenzyl 2-methylhex-3-yl ester

Inchi: InChI=1S/C19H26N2O8/c1-5-6-17(12(2)3)29-19(23)8-7-18(22)28-11-14-9-15(20(24)25)1

InchiKey: BZYDWRORUAESON-UHFFFAOYSA-N

Formula: C19H26N2O8

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

Mol. weight [g/mol]: 410.42

Physical Properties

Property code	Value	Unit	Source
gf	-209.00	kJ/mol	Joback Method
hf	-755.05	kJ/mol	Joback Method
hfus	59.09	kJ/mol	Joback Method
hvap	112.87	kJ/mol	Joback Method
log10ws	-6.33		Crippen Method
logp	4.003		Crippen Method
mcvol	304.530	ml/mol	McGowan Method
pc	1452.35	kPa	Joback Method
rinpol	2805.00		NIST Webbook
rinpol	2805.00		NIST Webbook
tb	1131.12	K	Joback Method
tc	1386.16	K	Joback Method
tf	769.41	K	Joback Method
vc	1.192	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1014.06	J/mol×K	1131.12	Joback Method
cpg	1021.32	J/mol×K	1173.63	Joback Method
cpg	1026.87	J/mol×K	1216.13	Joback Method
cpg	1030.75	J/mol×K	1258.64	Joback Method
cpg	1032.98	J/mol×K	1301.15	Joback Method
cpg	1033.60	J/mol×K	1343.65	Joback Method
cpg	1032.66	J/mol×K	1386.16	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382238&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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