

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

<b>Inchi:</b>	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
<b>InchiKey:</b>	GXTUOVGSHGTMSD-UHFFFAOYSA-N
<b>Formula:</b>	C19H26N2O8
<b>SMILES:</b>	CCCC(OC(=O)CCC(=O)OCc1cc([N+](=O)[O-])cc([N+](=O)[O-])c1C)C(C)C
<b>Mol. weight [g/mol]:</b>	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
mvol	304.530	ml/mol	McGowan Method
pc	1452.35	kPa	Joback Method
rinpol	2886.00		NIST Webbook
rinpol	2886.00		NIST Webbook
tb	1131.12	K	Joback Method
tc	1386.16	K	Joback Method
tf	769.41	K	Joback Method
vc	1.192	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

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

# Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U381009&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U381009&amp;Units=SI</a>

# Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpola:</b>	Non-polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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