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

Inchi: InChI=1S/C19H26N2O8/c1-3-4-5-6-7-10-28-18(22)8-9-19(23)29-13-15-11-16(20(24)25)1

InchiKey: XJXGJUSOMNJDCR-UHFFFAOYSA-N

Formula: C19H26N2O8

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

Mol. weight [g/mol]: 410.42

Physical Properties

Property code	Value	Unit	Source
gf	-204.12	kJ/mol	Joback Method
hf	-744.49	kJ/mol	Joback Method
hfus	66.14	kJ/mol	Joback Method
hvap	113.64	kJ/mol	Joback Method
log10ws	-6.46		Crippen Method
logp	4.148		Crippen Method
mcvol	304.530	ml/mol	McGowan Method
pc	1434.80	kPa	Joback Method
rinpol	3032.00		NIST Webbook
rinpol	3032.00		NIST Webbook
tb	1132.00	K	Joback Method
tc	1386.20	K	Joback Method
tf	799.41	K	Joback Method
vc	1.204	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1013.84	J/mol×K	1132.00	Joback Method
cpg	1021.34	J/mol×K	1174.37	Joback Method
cpg	1027.17	J/mol×K	1216.73	Joback Method
cpg	1031.38	J/mol×K	1259.10	Joback Method
cpg	1033.99	J/mol×K	1301.47	Joback Method
cpg	1035.04	J/mol×K	1343.83	Joback Method
cpg	1034.57	J/mol×K	1386.20	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U381011&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