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

Inchi: InChI=1S/C16H20N2O8/c1-3-4-7-25-15(19)5-6-16(20)26-10-12-8-13(17(21)22)9-14(11(1

InchiKey: RZASFLGGUQLWBK-UHFFFAOYSA-N

Formula: C16H20N2O8

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

Mol. weight [g/mol]: 368.34

Physical Properties

Property code	Value	Unit	Source
gf	-229.38	kJ/mol	Joback Method
hf	-682.57	kJ/mol	Joback Method
hfus	58.37	kJ/mol	Joback Method
hvap	106.97	kJ/mol	Joback Method
log10ws	-5.20		Crippen Method
logp	2.978		Crippen Method
mcvol	262.260	ml/mol	McGowan Method
pc	1807.70	kPa	Joback Method
rinpol	2743.00		NIST Webbook
rinpol	2743.00		NIST Webbook
tb	1063.36	K	Joback Method
tc	1309.78	K	Joback Method
tf	765.60	K	Joback Method
vc	1.036	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	839.34	J/mol×K	1063.36	Joback Method
cpg	846.98	J/mol×K	1104.43	Joback Method
cpg	853.16	J/mol×K	1145.50	Joback Method
cpg	857.88	J/mol×K	1186.57	Joback Method
cpg	861.17	J/mol×K	1227.64	Joback Method
cpg	863.04	J/mol×K	1268.71	Joback Method
cpg	863.51	J/mol×K	1309.78	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U381007&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