Succinic acid, 3,5-dinitro-4-methylbenzyl isobutyl ester

Inchi: InChI=1S/C16H20N2O8/c1-10(2)8-25-15(19)4-5-16(20)26-9-12-6-13(17(21)22)11(3)14(7

InchiKey: FMFVSXJIJORMRO-UHFFFAOYSA-N

Formula: C16H20N2O8

SMILES: Cc1c([N+](=O)[O-])cc(COC(=O)CCC(=O)OCC(C)C)cc1[N+](=O)[O-]

Mol. weight [g/mol]: 368.34

Physical Properties

Property code	Value	Unit	Source
gf	-231.82	kJ/mol	Joback Method
hf	-687.85	kJ/mol	Joback Method
hfus	54.84	kJ/mol	Joback Method
hvap	106.58	kJ/mol	Joback Method
log10ws	-4.96		Crippen Method
logp	2.834		Crippen Method
mcvol	262.260	ml/mol	McGowan Method
pc	1820.06	kPa	Joback Method
rinpol	2615.00		NIST Webbook
rinpol	2615.00		NIST Webbook
tb	1062.92	K	Joback Method
tc	1310.98	K	Joback Method
tf	750.60	K	Joback Method
vc	1.030	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	839.65	J/mol×K	1062.92	Joback Method
cpg	847.24	J/mol×K	1104.26	Joback Method
cpg	853.32	J/mol×K	1145.61	Joback Method
cpg	857.92	J/mol×K	1186.95	Joback Method
cpg	861.04	J/mol×K	1228.29	Joback Method
cpg	862.72	J/mol×K	1269.63	Joback Method
cpg	862.96	J/mol×K	1310.98	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382236&Units=SI

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