Succinic acid, 3,5-dinitrobenzyl isobutyl ester

Inchi: InChI=1S/C15H18N2O8/c1-10(2)8-24-14(18)3-4-15(19)25-9-11-5-12(16(20)21)7-13(6-11
InchiKey: FXSUKLDBWMXNKE-UHFFFAOYSA-N
Formula: C15H18N2O8
SMILES: CC(C)COC(=O)CCC(=O)OCc1cc([N+](=O)[O-])cc([N+](=O)[O-])c1
Mol. weight [g/mol]: 354.31

Physical Properties

Property code	Value	Unit	Source
gf	-230.61	kJ/mol	Joback Method
hf	-655.74	kJ/mol	Joback Method
hfus	52.64	kJ/mol	Joback Method
hvap	103.69	kJ/mol	Joback Method
log10ws	-4.48		Crippen Method
logp	2.526		Crippen Method
mcvol	248.170	ml/mol	McGowan Method
pc	2005.50	kPa	Joback Method
rinpol	2615.00		NIST Webbook
rinpol	2615.00		NIST Webbook
tb	1035.06	K	Joback Method
tc	1282.22	K	Joback Method
tf	726.81	K	Joback Method
vc	0.974	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	784.40	J/mol×K	1035.06	Joback Method
cpg	792.21	J/mol×K	1076.25	Joback Method
cpg	798.61	J/mol×K	1117.45	Joback Method
cpg	803.63	J/mol×K	1158.64	Joback Method
cpg	807.30	J/mol×K	1199.83	Joback Method
cpg	809.62	J/mol×K	1241.03	Joback Method
cpg	810.63	J/mol×K	1282.22	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=U381092&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