Succinic acid, butyl 3,5-dinitrobenzyl ester

Inchi: InChI=1S/C15H18N2O8/c1-2-3-6-24-14(18)4-5-15(19)25-10-11-7-12(16(20)21)9-13(8-11
InchiKey: HBMUKYXEIGYSML-UHFFFAOYSA-N
Formula: C15H18N2O8
SMILES: CCCCOC(=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	-228.17	kJ/mol	Joback Method
hf	-650.46	kJ/mol	Joback Method
hfus	56.16	kJ/mol	Joback Method
hvap	104.08	kJ/mol	Joback Method
log10ws	-4.73		Crippen Method
logp	2.670		Crippen Method
mcvol	248.170	ml/mol	McGowan Method
pc	1991.21	kPa	Joback Method
rinpol	2665.00		NIST Webbook
rinpol	2665.00		NIST Webbook
tb	1035.50	K	Joback Method
tc	1280.58	K	Joback Method
tf	741.81	K	Joback Method
vc	0.980	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	784.03	J/mol×K	1035.50	Joback Method
cpg	791.86	J/mol×K	1076.35	Joback Method
cpg	798.34	J/mol×K	1117.19	Joback Method
cpg	803.47	J/mol×K	1158.04	Joback Method
cpg	807.27	J/mol×K	1198.89	Joback Method
cpg	809.78	J/mol×K	1239.74	Joback Method
cpg	811.02	J/mol×K	1280.58	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=U381093&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