Succinic acid, 3-nitrobenzyl propyl ester

Inchi: InChI=1S/C14H17NO6/c1-2-8-20-13(16)6-7-14(17)21-10-11-4-3-5-12(9-11)15(18)19/h3-5
InchiKey: KAHAOAKFRGEJRU-UHFFFAOYSA-N
Formula: C14H17NO6
SMILES: CCCOC(=O)CCC(=O)OCc1cccc([N+](=O)[O-])c1
Mol. weight [g/mol]: 295.29

Physical Properties

Property code	Value	Unit	Source
gf	-262.51	kJ/mol	Joback Method
hf	-607.59	kJ/mol	Joback Method
hfus	42.60	kJ/mol	Joback Method
hvap	84.60	kJ/mol	Joback Method
log10ws	-3.66		Crippen Method
logp	2.371		Crippen Method
mcvol	216.660	ml/mol	McGowan Method
pc	2179.52	kPa	Joback Method
rinpol	2283.00		NIST Webbook
rinpol	2283.00		NIST Webbook
tb	855.80	K	Joback Method
tc	1081.29	K	Joback Method
tf	574.41	K	Joback Method
vc	0.842	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	642.35	J/mol×K	855.80	Joback Method
cpg	654.06	J/mol×K	893.38	Joback Method
cpg	664.66	J/mol×K	930.96	Joback Method
cpg	674.17	J/mol×K	968.55	Joback Method
cpg	682.61	J/mol×K	1006.13	Joback Method
cpg	689.98	J/mol×K	1043.71	Joback Method
cpg	696.31	J/mol×K	1081.29	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=U381686&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