Succinic acid, ethyl 3-methyl-4-nitrobenzyl ester

Inchi: InChI=1S/C14H17NO6/c1-3-20-13(16)6-7-14(17)21-9-11-4-5-12(15(18)19)10(2)8-11/h4-5

InchiKey: JOEQXCQSDJEHEZ-UHFFFAOYSA-N

Formula: C14H17NO6

SMILES: CCOC(=O)CCC(=O)OCc1ccc([N+](=O)[O-])c(C)c1

Mol. weight [g/mol]: 295.29

Physical Properties

Property code	Value	Unit	Source
gf	-272.14	kJ/mol	Joback Method
hf	-619.06	kJ/mol	Joback Method
hfus	42.21	kJ/mol	Joback Method
hvap	85.26	kJ/mol	Joback Method
log10ws	-3.71		Crippen Method
logp	2.290		Crippen Method
mcvol	216.660	ml/mol	McGowan Method
pc	2149.31	kPa	Joback Method
rinpol	2256.00		NIST Webbook
rinpol	2256.00		NIST Webbook
tb	860.78	K	Joback Method
tc	1087.02	K	Joback Method
tf	586.93	K	Joback Method
vc	0.842	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	640.86	J/mol×K	860.78	Joback Method
cpg	652.48	J/mol×K	898.49	Joback Method
cpg	662.99	J/mol×K	936.19	Joback Method
cpg	672.40	J/mol×K	973.90	Joback Method
cpg	680.70	J/mol×K	1011.60	Joback Method
cpg	687.92	J/mol×K	1049.31	Joback Method
cpg	694.05	J/mol×K	1087.02	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=U380977&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