

Succinic acid, ethyl 3-methyl-2-nitrobenzyl ester

Inchi:	InChI=1S/C14H17NO6/c1-3-20-12(16)7-8-13(17)21-9-11-6-4-5-10(2)14(11)15(18)19/h4-13
InchiKey:	IVPOKIKLIPUSIP-UHFFFAOYSA-N
Formula:	C14H17NO6
SMILES:	CCOC(=O)CCC(=O)OCc1cccc(C)c1[N+](=O)[O-]
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
mvol	216.660	ml/mol	McGowan Method
pc	2149.31	kPa	Joback Method
rinpol	2154.00		NIST Webbook
rinpol	2154.00		NIST Webbook
tb	860.78	K	Joback Method
tc	1087.02	K	Joback Method
tf	586.93	K	Joback Method
vc	0.842	m ³ /kmol	Joback Method

Temperature Dependent Properties

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

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=U380964&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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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