

Succinic acid, hexyl 3-nitrobenzyl ester

Inchi:	InChI=1S/C17H23NO6/c1-2-3-4-5-11-23-16(19)9-10-17(20)24-13-14-7-6-8-15(12-14)18(
InchiKey:	MMGXWORDSWFKSC-UHFFFAOYSA-N
Formula:	C17H23NO6
SMILES:	CCCCCOC(=O)CCC(=O)OCc1cccc([N+](=O)[O-])c1
Mol. weight [g/mol]:	337.37

Physical Properties

Property code	Value	Unit	Source
gf	-237.25	kJ/mol	Joback Method
hf	-669.51	kJ/mol	Joback Method
hfus	50.37	kJ/mol	Joback Method
hvap	91.28	kJ/mol	Joback Method
log10ws	-4.91		Crippen Method
logp	3.542		Crippen Method
mcvol	258.930	ml/mol	McGowan Method
pc	1693.51	kPa	Joback Method
rinpol	2578.00		NIST Webbook
rinpol	2578.00		NIST Webbook
tb	924.44	K	Joback Method
tc	1146.52	K	Joback Method
tf	608.22	K	Joback Method
vc	1.010	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	812.38	J/molxK	924.44	Joback Method
cpg	824.62	J/molxK	961.45	Joback Method
cpg	835.65	J/molxK	998.47	Joback Method
cpg	845.49	J/molxK	1035.48	Joback Method
cpg	854.17	J/molxK	1072.49	Joback Method
cpg	861.72	J/molxK	1109.51	Joback Method
cpg	868.15	J/molxK	1146.52	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U381691&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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
hvpap:	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
rinppl:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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