

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

Inchi:	InChI=1S/C17H23NO6/c1-3-4-5-10-23-16(19)8-9-17(20)24-12-14-6-7-15(18(21)22)13(2)
InchiKey:	WBLRFTVGWPQFGJ-UHFFFAOYSA-N
Formula:	C17H23NO6
SMILES:	CCCCCOC(=O)CCC(=O)OCc1ccc([N+](=O)[O-])c(C)c1
Mol. weight [g/mol]:	337.37

Physical Properties

Property code	Value	Unit	Source
gf	-246.88	kJ/mol	Joback Method
hf	-680.98	kJ/mol	Joback Method
hfus	49.98	kJ/mol	Joback Method
hvap	91.94	kJ/mol	Joback Method
log10ws	-4.97		Crippen Method
logp	3.460		Crippen Method
mvol	258.930	ml/mol	McGowan Method
pc	1672.79	kPa	Joback Method
rinpol	2548.00		NIST Webbook
rinpol	2548.00		NIST Webbook
tb	929.42	K	Joback Method
tc	1152.32	K	Joback Method
tf	620.74	K	Joback Method
vc	1.010	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	811.03	J/molxK	929.42	Joback Method
cpg	823.17	J/molxK	966.57	Joback Method
cpg	834.07	J/molxK	1003.72	Joback Method
cpg	843.77	J/molxK	1040.87	Joback Method
cpg	852.26	J/molxK	1078.02	Joback Method
cpg	859.58	J/molxK	1115.17	Joback Method
cpg	865.74	J/molxK	1152.32	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=U380981&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

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

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