

Succinic acid, 2-methylpent-3-yl 3-nitrobenzyl ester

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

Physical Properties

Property code	Value	Unit	Source
gf	-242.13	kJ/mol	Joback Method
hf	-680.07	kJ/mol	Joback Method
hfus	43.33	kJ/mol	Joback Method
hvap	90.50	kJ/mol	Joback Method
log10ws	-4.78		Crippen Method
logp	3.396		Crippen Method
mvol	258.930	ml/mol	McGowan Method
pc	1716.03	kPa	Joback Method
rinpol	2513.00		NIST Webbook
rinpol	2513.00		NIST Webbook
tb	923.56	K	Joback Method
tc	1150.00	K	Joback Method
tf	578.22	K	Joback Method
vc	0.998	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	813.39	J/mol×K	923.56	Joback Method
cpg	825.78	J/mol×K	961.30	Joback Method
cpg	836.89	J/mol×K	999.04	Joback Method
cpg	846.73	J/mol×K	1036.78	Joback Method
cpg	855.34	J/mol×K	1074.52	Joback Method
cpg	862.75	J/mol×K	1112.26	Joback Method
cpg	868.97	J/mol×K	1150.00	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=U390179&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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