Succinic acid, 4-methoxy-3-nitrobenzyl 2-methylhex-3-yl ester

Inchi: InChI=1S/C19H27NO7/c1-5-6-16(13(2)3)27-19(22)10-9-18(21)26-12-14-7-8-17(25-4)15(

InchiKey: XBLWESJOPLAZNK-UHFFFAOYSA-N

Formula: C19H27NO7

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

Mol. weight [g/mol]: 381.42

Physical Properties

Property code	Value	Unit	Source
gf	-339.92	kJ/mol	Joback Method
hf	-865.04	kJ/mol	Joback Method
hfus	49.31	kJ/mol	Joback Method
hvap	98.02	kJ/mol	Joback Method
log10ws	-5.32		Crippen Method
logp	3.795		Crippen Method
mcvol	292.980	ml/mol	McGowan Method
pc	1436.98	kPa	Joback Method
rinpol	2784.00		NIST Webbook
rinpol	2784.00		NIST Webbook
tb	996.72	K	Joback Method
tc	1225.89	K	Joback Method
tf	635.51	K	Joback Method
vc	1.127	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	954.76	J/mol×K	996.72	Joback Method
cpg	966.12	J/mol×K	1034.91	Joback Method
cpg	975.92	J/mol×K	1073.11	Joback Method
cpg	984.16	J/mol×K	1111.30	Joback Method
cpg	990.84	J/mol×K	1149.50	Joback Method
cpg	995.99	J/mol×K	1187.69	Joback Method
cpg	999.60	J/mol×K	1225.89	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U380951&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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