Succinic acid, heptyl 4-methoxy-3-nitrobenzyl ester

Inchi: InChI=1S/C19H27NO7/c1-3-4-5-6-7-12-26-18(21)10-11-19(22)27-14-15-8-9-17(25-2)16(

InchiKey: WLYRVJRUJSHFDQ-UHFFFAOYSA-N

Formula: C19H27NO7

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

Mol. weight [g/mol]: 381.42

Physical Properties

Property code	Value	Unit	Source
gf	-335.04	kJ/mol	Joback Method
hf	-854.48	kJ/mol	Joback Method
hfus	56.35	kJ/mol	Joback Method
hvap	98.80	kJ/mol	Joback Method
log10ws	-5.45		Crippen Method
logp	3.940		Crippen Method
mcvol	292.980	ml/mol	McGowan Method
pc	1419.71	kPa	Joback Method
rinpol	2919.00		NIST Webbook
rinpol	2919.00		NIST Webbook
tb	997.60	K	Joback Method
tc	1224.60	K	Joback Method
tf	665.51	K	Joback Method
vc	1.139	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	953.95	J/mol×K	997.60	Joback Method
cpg	965.34	J/mol×K	1035.43	Joback Method
cpg	975.22	J/mol×K	1073.27	Joback Method
cpg	983.60	J/mol×K	1111.10	Joback Method
cpg	990.48	J/mol×K	1148.93	Joback Method
cpg	995.88	J/mol×K	1186.76	Joback Method
cpg	999.80	J/mol×K	1224.60	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=U380953&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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