Succinic acid, 2-methylhex-3-yl 3-methyl-2-nitrobenzyl ester

Inchi: InChI=1S/C19H27NO6/c1-5-7-16(13(2)3)26-18(22)11-10-17(21)25-12-15-9-6-8-14(4)19(
InchiKey: UHNVYUWZFYECNJ-UHFFFAOYSA-N
Formula: C19H27NO6
SMILES: CCCC(OC(=O)CCC(=O)OCc1cccc(C)c1[N+](=O)[O-])C(C)C
Mol. weight [g/mol]: 365.42

Physical Properties

Property code	Value	Unit	Source
gf	-234.92	kJ/mol	Joback Method
hf	-732.82	kJ/mol	Joback Method
hfus	48.12	kJ/mol	Joback Method
hvap	95.61	kJ/mol	Joback Method
log10ws	-5.68		Crippen Method
logp	4.095		Crippen Method
mcvol	287.110	ml/mol	McGowan Method
pc	1455.68	kPa	Joback Method
rinpol	2506.00		NIST Webbook
rinpol	2506.00		NIST Webbook
tb	974.30	K	Joback Method
tc	1201.77	K	Joback Method
tf	613.28	K	Joback Method
vc	1.109	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	928.74	J/mol×K	974.30	Joback Method
cpg	941.13	J/mol×K	1012.21	Joback Method
cpg	952.13	J/mol×K	1050.12	Joback Method
cpg	961.77	J/mol×K	1088.03	Joback Method
cpg	970.07	J/mol×K	1125.95	Joback Method
cpg	977.05	J/mol×K	1163.86	Joback Method
cpg	982.75	J/mol×K	1201.77	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=U380968&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