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

Inchi: InChI=1S/C19H28O4/c1-4-17(15(2)3)23-19(21)13-12-18(20)22-14-8-11-16-9-6-5-7-10-16
InchiKey: JXXRZJVYNRCMMC-UHFFFAOYSA-N
Formula: C19H28O4
SMILES: CCC(OC(=O)CCC(=O)OCCCc1ccccc1)C(C)C
Mol. weight [g/mol]: 320.42

Physical Properties

Property code	Value	Unit	Source
gf	-251.21	kJ/mol	Joback Method
hf	-699.12	kJ/mol	Joback Method
hfus	37.53	kJ/mol	Joback Method
hvap	77.70	kJ/mol	Joback Method
log10ws	-4.47		Crippen Method
logp	3.920		Crippen Method
mcvol	269.690	ml/mol	McGowan Method
pc	1475.88	kPa	Joback Method
rinpol	2272.00		NIST Webbook
rinpol	2272.00		NIST Webbook
tb	812.50	K	Joback Method
tc	1015.45	K	Joback Method
tf	444.63	K	Joback Method
vc	1.028	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	820.77	J/mol×K	812.50	Joback Method
cpg	837.10	J/mol×K	846.32	Joback Method
cpg	852.27	J/mol×K	880.15	Joback Method
cpg	866.32	J/mol×K	913.97	Joback Method
cpg	879.27	J/mol×K	947.80	Joback Method
cpg	891.14	J/mol×K	981.62	Joback Method
cpg	901.96	J/mol×K	1015.45	Joback Method
dvisc	0.0010535	Pa×s	444.63	Joback Method

dvisc	0.0004721	Pa×s	505.94	Joback Method
dvisc	0.0002516	Pa×s	567.25	Joback Method
dvisc	0.0001517	Pa×s	628.57	Joback Method
dvisc	0.0001000	Pa×s	689.88	Joback Method
dvisc	0.0000706	Pa×s	751.19	Joback Method
dvisc	0.0000525	Pa×s	812.50	Joback Method

Sources

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=U389724&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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

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