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

Inchi: InChI=1S/C18H26O4/c1-14(2)15(3)22-18(20)12-11-17(19)21-13-7-10-16-8-5-4-6-9-16/h4

InchiKey: MNBLNZOXQXAZAS-UHFFFAOYSA-N

Formula: C18H26O4

SMILES: CC(C)C(C)OC(=O)CCC(=O)OCCCc1ccccc1

Mol. weight [g/mol]: 306.40

Physical Properties

Property code	Value	Unit	Source
gf	-259.63	kJ/mol	Joback Method
hf	-678.48	kJ/mol	Joback Method
hfus	34.94	kJ/mol	Joback Method
hvap	75.47	kJ/mol	Joback Method
log10ws	-4.06		Crippen Method
logp	3.530		Crippen Method
mcvol	255.600	ml/mol	McGowan Method
pc	1591.08	kPa	Joback Method
rinpol	2188.00		NIST Webbook
tb	789.62	K	Joback Method
tc	993.35	K	Joback Method
tf	433.36	K	Joback Method
vc	0.972	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	763.01	J/mol×K	789.62	Joback Method
cpg	832.79	J/mol×K	959.40	Joback Method
cpg	820.99	J/mol×K	925.44	Joback Method
cpg	808.13	J/mol×K	891.49	Joback Method
cpg	794.20	J/mol×K	857.53	Joback Method
cpg	779.16	J/mol×K	823.58	Joback Method
cpg	843.56	J/mol×K	993.35	Joback Method
dvisc	0.0000604	Pa×s	789.62	Joback Method
dvisc	0.0000810	Pa×s	730.24	Joback Method

dvisc	0.0001144	Pa×s	670.87	Joback Method
dvisc	0.0001729	Pa×s	611.49	Joback Method
dvisc	0.0002855	Pa×s	552.11	Joback Method
dvisc	0.0005318	Pa×s	492.74	Joback Method
dvisc	0.0011751	Pa×s	433.36	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U389723&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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