Succinic acid, 2,3-dimethylphenyl isobutyl ester

Inchi: InChI=1S/C16H22O4/c1-11(2)10-19-15(17)8-9-16(18)20-14-7-5-6-12(3)13(14)4/h5-7,11H

InchiKey: LRNXBYPGZPCXKY-UHFFFAOYSA-N

Formula: C16H22O4

SMILES: Cc1cccc(OC(=O)CCC(=O)OCC(C)C)c1C

Mol. weight [g/mol]: 278.34

Physical Properties

Property code	Value	Unit	Source
gf	-293.29	kJ/mol	Joback Method
hf	-654.86	kJ/mol	Joback Method
hfus	32.51	kJ/mol	Joback Method
hvap	72.73	kJ/mol	Joback Method
log10ws	-3.87		Crippen Method
logp	3.188		Crippen Method
mcvol	227.420	ml/mol	McGowan Method
pc	1806.16	kPa	Joback Method
rinpol	2022.00		NIST Webbook
tb	754.26	K	Joback Method
tc	959.78	K	Joback Method
tf	450.86	K	Joback Method
vc	0.866	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	648.19	J/mol×K	754.26	Joback Method
cpg	663.44	J/mol×K	788.51	Joback Method
cpg	677.69	J/mol×K	822.77	Joback Method
cpg	690.94	J/mol×K	857.02	Joback Method
cpg	703.22	J/mol×K	891.28	Joback Method
cpg	714.52	J/mol×K	925.53	Joback Method
cpg	724.85	J/mol×K	959.78	Joback Method
dvisc	0.0008196	Pa×s	450.86	Joback Method
dvisc	0.0004662	Pa×s	501.43	Joback Method

dvisc	0.0002941	Pa×s	551.99	Joback Method
dvisc	0.0002004	Pa×s	602.56	Joback Method
dvisc	0.0001449	Pa×s	653.13	Joback Method
dvisc	0.0001098	Pa×s	703.69	Joback Method
dvisc	0.0000864	Pa×s	754.26	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=U349620&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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