

Succinic acid, di(1-tert-butoxyprop-2-yl) ester

Inchi: InChI=1S/C17H32O6/c1-9-15(23-17(6,7)8)21-14(19)11-10-13(18)20-12(2)22-16(3,4)5/h1
InchiKey: GSUXOVAYUKRKIB-UHFFFAOYSA-N
Formula: C17H32O6
SMILES: CCC(OC(=O)CCC(=O)OC(C)OC(C)(C)C)OC(C)(C)C
Mol. weight [g/mol]: 332.43

Physical Properties

Property code	Value	Unit	Source
gf	-584.78	kJ/mol	Joback Method
hf	-1176.31	kJ/mol	Joback Method
hfus	25.86	kJ/mol	Joback Method
hvap	73.20	kJ/mol	Joback Method
log10ws	-4.28		Crippen Method
logp	3.565		Crippen Method
mcvol	277.010	ml/mol	McGowan Method
pc	1333.93	kPa	Joback Method
rinpol	1934.00		NIST Webbook
rinpol	1934.00		NIST Webbook
tb	778.44	K	Joback Method
tc	971.19	K	Joback Method
tf	444.97	K	Joback Method
vc	1.038	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	855.99	J/molxK	778.44	Joback Method
cpg	873.13	J/molxK	810.57	Joback Method
cpg	889.17	J/molxK	842.69	Joback Method
cpg	904.13	J/molxK	874.82	Joback Method
cpg	918.02	J/molxK	906.94	Joback Method
cpg	930.86	J/molxK	939.07	Joback Method
cpg	942.68	J/molxK	971.19	Joback Method
dvisc	0.0007099	Paxs	444.97	Joback Method

dvisc	0.0003003	Paxs	500.55	Joback Method
dvisc	0.0001508	Paxs	556.13	Joback Method
dvisc	0.0000859	Paxs	611.71	Joback Method
dvisc	0.0000537	Paxs	667.28	Joback Method
dvisc	0.0000361	Paxs	722.86	Joback Method
dvisc	0.0000257	Paxs	778.44	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=U382462&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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