

Succinic acid, ethyl 1-tert-butoxyprop-2-yl ester

Inchi:	InChI=1S/C13H24O5/c1-6-12(18-13(3,4)5)17-11(15)9-8-10(14)16-7-2/h12H,6-9H2,1-5H3
InchiKey:	GWIFANGOIJHJB-UHFFFAOYSA-N
Formula:	C13H24O5
SMILES:	CCOC(=O)CCC(=O)OC(CC)OC(C)(C)C
Mol. weight [g/mol]:	260.33

Physical Properties

Property code	Value	Unit	Source
gf	-513.86	kJ/mol	Joback Method
hf	-947.50	kJ/mol	Joback Method
hfus	25.25	kJ/mol	Joback Method
hvap	63.57	kJ/mol	Joback Method
log10ws	-2.80		Crippen Method
logp	2.424		Crippen Method
mvol	214.780	ml/mol	McGowan Method
pc	1789.39	kPa	Joback Method
rinpol	1569.00		NIST Webbook
rinpol	1569.00		NIST Webbook
tb	668.17	K	Joback Method
tc	854.57	K	Joback Method
tf	390.24	K	Joback Method
vc	0.812	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	599.63	J/molxK	668.17	Joback Method
cpg	615.26	J/molxK	699.24	Joback Method
cpg	630.08	J/molxK	730.30	Joback Method
cpg	644.10	J/molxK	761.37	Joback Method
cpg	657.32	J/molxK	792.44	Joback Method
cpg	669.74	J/molxK	823.51	Joback Method
cpg	681.38	J/molxK	854.57	Joback Method
dvisc	0.0014313	Paxs	390.24	Joback Method

dvisc	0.0006922	Paxs	436.56	Joback Method
dvisc	0.0003849	Paxs	482.88	Joback Method
dvisc	0.0002371	Paxs	529.21	Joback Method
dvisc	0.0001580	Paxs	575.53	Joback Method
dvisc	0.0001118	Paxs	621.85	Joback Method
dvisc	0.0000830	Paxs	668.17	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=U382452&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cp_g:	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:	Log ₁₀ 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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