

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

Inchi:	InChI=1S/C17H32O5/c1-6-8-9-10-13-20-14(18)11-12-15(19)21-16(7-2)22-17(3,4)5/h16H
InchiKey:	NBDJEPWZBSVRQB-UHFFFAOYSA-N
Formula:	C17H32O5
SMILES:	CCCCCOC(=O)CCC(=O)OC(CC)OC(C)(C)C
Mol. weight [g/mol]:	316.43

Physical Properties

Property code	Value	Unit	Source
gf	-480.18	kJ/mol	Joback Method
hf	-1030.06	kJ/mol	Joback Method
hfus	35.61	kJ/mol	Joback Method
hvap	72.47	kJ/mol	Joback Method
log10ws	-4.47		Crippen Method
logp	3.984		Crippen Method
mvol	271.140	ml/mol	McGowan Method
pc	1324.24	kPa	Joback Method
rinpol	1942.00		NIST Webbook
rinpol	1942.00		NIST Webbook
tb	759.69	K	Joback Method
tc	944.40	K	Joback Method
tf	435.32	K	Joback Method
vc	1.036	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	823.69	J/molxK	759.69	Joback Method
cpg	840.79	J/molxK	790.47	Joback Method
cpg	856.91	J/molxK	821.26	Joback Method
cpg	872.07	J/molxK	852.04	Joback Method
cpg	886.28	J/molxK	882.83	Joback Method
cpg	899.55	J/molxK	913.61	Joback Method
cpg	911.90	J/molxK	944.40	Joback Method
dvisc	0.0009176	Paxs	435.32	Joback Method

dvisc	0.0004234	Paxs	489.38	Joback Method
dvisc	0.0002278	Paxs	543.44	Joback Method
dvisc	0.0001372	Paxs	597.50	Joback Method
dvisc	0.0000898	Paxs	651.57	Joback Method
dvisc	0.0000628	Paxs	705.63	Joback Method
dvisc	0.0000462	Paxs	759.69	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=U382457&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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