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

Inchi: InChI=1S/C15H28O5/c1-7-14(20-15(4,5)6)19-13(17)9-8-12(16)18-10-11(2)3/h11,14H,7-1

InchiKey: WTKPGSIDIVANHI-UHFFFAOYSA-N

Formula: C15H28O5

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

Mol. weight [g/mol]: 288.38

Physical Properties

Property code	Value	Unit	Source
gf	-499.46	kJ/mol	Joback Method
hf	-994.06	kJ/mol	Joback Method
hfus	26.91	kJ/mol	Joback Method
hvap	67.63	kJ/mol	Joback Method
log10ws	-3.39		Crippen Method
logp	3.060		Crippen Method
mcvol	242.960	ml/mol	McGowan Method
pc	1540.29	kPa	Joback Method
rinpol	1708.00		NIST Webbook
rinpol	1708.00		NIST Webbook
tb	713.49	K	Joback Method
tc	900.48	K	Joback Method
tf	397.78	K	Joback Method
vc	0.918	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	709.89	J/mol×K	713.49	Joback Method
cpg	784.11	J/mol×K	869.31	Joback Method
cpg	771.07	J/mol×K	838.15	Joback Method
cpg	757.14	J/mol×K	806.98	Joback Method
cpg	742.31	J/mol×K	775.82	Joback Method
cpg	726.56	J/mol×K	744.65	Joback Method
cpg	796.26	J/mol×K	900.48	Joback Method
dvisc	0.0000575	Pa×s	713.49	Joback Method

dvisc	0.0000795	Pa×s	660.87	Joback Method
dvisc	0.0001161	Pa×s	608.25	Joback Method
dvisc	0.0001823	Pa×s	555.63	Joback Method
dvisc	0.0003146	Pa×s	503.02	Joback Method
dvisc	0.0006167	Pa×s	450.40	Joback Method
dvisc	0.0014443	Pa×s	397.78	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382454&Units=SI

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