Glutaric acid, 1-(tert-butoxy)prop-2-yl ethyl ester

Inchi: InChI=1S/C14H26O5/c1-6-17-12(15)8-7-9-13(16)19-11(2)10-18-14(3,4)5/h11H,6-10H2,1

InchiKey: WFVYQHFGTZCXDU-UHFFFAOYSA-N

Formula: C14H26O5

SMILES: CCOC(=O)CCCC(=O)OC(C)COC(C)(C)C

Mol. weight [g/mol]: 274.35

Physical Properties

Property code	Value	Unit	Source
gf	-505.44	kJ/mol	Joback Method
hf	-968.14	kJ/mol	Joback Method
hfus	27.84	kJ/mol	Joback Method
hvap	65.80	kJ/mol	Joback Method
log10ws	-2.72		Crippen Method
logp	2.467		Crippen Method
mcvol	228.870	ml/mol	McGowan Method
pc	1652.46	kPa	Joback Method
rinpol	1849.00		NIST Webbook
rinpol	1849.00		NIST Webbook
tb	691.05	K	Joback Method
tc	876.32	K	Joback Method
tf	401.51	K	Joback Method
vc	0.869	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	653.91	J/mol×K	691.05	Joback Method
cpg	725.75	J/mol×K	845.44	Joback Method
cpg	713.06	J/mol×K	814.56	Joback Method
cpg	699.53	J/mol×K	783.68	Joback Method
cpg	685.17	J/mol×K	752.81	Joback Method
cpg	669.96	J/mol×K	721.93	Joback Method
cpg	737.63	J/mol×K	876.32	Joback Method
dvisc	0.0000720	Pa×s	691.05	Joback Method

dvisc	0.0000972	Pa×s	642.79	Joback Method
dvisc	0.0001378	Pa×s	594.54	Joback Method
dvisc	0.0002078	Pa×s	546.28	Joback Method
dvisc	0.0003394	Pa×s	498.02	Joback Method
dvisc	0.0006159	Pa×s	449.77	Joback Method
dvisc	0.0012897	Pa×s	401.51	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=U380527&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

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