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

Inchi: InChI=1S/C16H30O5/c1-7-12(2)20-14(17)9-8-10-15(18)21-13(3)11-19-16(4,5)6/h12-13H

InchiKey: BWYZHBBQJLRAHG-UHFFFAOYSA-N

Formula: C16H30O5

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

Mol. weight [g/mol]: 302.41

Physical Properties

Property code	Value	Unit	Source
gf	-491.04	kJ/mol	Joback Method
hf	-1014.70	kJ/mol	Joback Method
hfus	29.50	kJ/mol	Joback Method
hvap	69.86	kJ/mol	Joback Method
log10ws	-3.67		Crippen Method
logp	3.245		Crippen Method
mcvol	257.050	ml/mol	McGowan Method
pc	1430.46	kPa	Joback Method
rinpol	2023.00		NIST Webbook
rinpol	2023.00		NIST Webbook
tb	736.37	K	Joback Method
tc	922.89	K	Joback Method
tf	409.05	K	Joback Method
vc	0.975	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	766.52	J/mol×K	736.37	Joback Method
cpg	783.51	J/mol×K	767.46	Joback Method
cpg	799.54	J/mol×K	798.54	Joback Method
cpg	814.61	J/mol×K	829.63	Joback Method
cpg	828.75	J/mol×K	860.71	Joback Method
cpg	841.95	J/mol×K	891.80	Joback Method
cpg	854.24	J/mol×K	922.89	Joback Method
dvisc	0.0012784	Pa×s	409.05	Joback Method

dvisc	0.0005406	Pa×s	463.60	Joback Method
dvisc	0.0002740	Pa×s	518.16	Joback Method
dvisc	0.0001581	Pa×s	572.71	Joback Method
dvisc	0.0001004	Pa×s	627.26	Joback Method
dvisc	0.0000685	Pa×s	681.82	Joback Method
dvisc	0.0000495	Pa×s	736.37	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=U380529&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