

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

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C19H36O6/c1-14(12-22-18(3,4)5)24-16(20)10-9-11-17(21)25-15(2)13-23-19(6)

KAGHLHQNPUPRR-UHFFFAOYSA-N

C19H36O6

CC(COC(C)(C)C)OC(=O)CCCC(=O)OC(C)COC(C)(C)C

360.49

Physical Properties

Property code	Value	Unit	Source
gf	-567.94	kJ/mol	Joback Method
hf	-1217.59	kJ/mol	Joback Method
hfus	31.04	kJ/mol	Joback Method
hvap	77.65	kJ/mol	Joback Method
log10ws	-4.12		Crippen Method
logp	3.650		Crippen Method
mcvol	305.190	ml/mol	McGowan Method
pc	1164.84	kPa	Joback Method
rinpol	2276.00		NIST Webbook
rinpol	2276.00		NIST Webbook
tb	824.20	K	Joback Method
tc	1018.23	K	Joback Method
tf	467.51	K	Joback Method
vc	1.149	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	974.27	J/mol×K	824.20	Joback Method
cpg	991.81	J/mol×K	856.54	Joback Method
cpg	1008.16	J/mol×K	888.88	Joback Method
cpg	1023.34	J/mol×K	921.21	Joback Method
cpg	1037.38	J/mol×K	953.55	Joback Method
cpg	1050.31	J/mol×K	985.89	Joback Method
cpg	1062.14	J/mol×K	1018.23	Joback Method
dvisc	0.0005324	Pa×s	467.51	Joback Method

dvisc	0.0002213	Pa×s	526.96	Joback Method
dvisc	0.0001100	Pa×s	586.41	Joback Method
dvisc	0.0000621	Pa×s	645.86	Joback Method
dvisc	0.0000386	Pa×s	705.30	Joback Method
dvisc	0.0000259	Pa×s	764.75	Joback Method
dvisc	0.0000184	Pa×s	824.20	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=U380545&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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