Diethylmalonic acid, propyl 1-tert-butyloxyprop-2-yl ester

Inchi: InChI=1S/C17H32O5/c1-8-11-20-14(18)17(9-2,10-3)15(19)22-13(4)12-21-16(5,6)7/h13H

InchiKey: KTTZEPZCXXYNEA-UHFFFAOYSA-N

Formula: C17H32O5

SMILES: CCCOC(=O)C(CC)(CC)C(=O)OC(C)COC(C)(C)C

Mol. weight [g/mol]: 316.43

Physical Properties

Property code	Value	Unit	Source
gf	-477.34	kJ/mol	Joback Method
hf	-1038.81	kJ/mol	Joback Method
hfus	28.20	kJ/mol	Joback Method
hvap	71.18	kJ/mol	Joback Method
log10ws	-3.73		Crippen Method
logp	3.493		Crippen Method
mcvol	271.140	ml/mol	McGowan Method
pc	1342.74	kPa	Joback Method
rinpol	1727.00		NIST Webbook
rinpol	1727.00		NIST Webbook
tb	756.46	K	Joback Method
tc	946.65	K	Joback Method
tf	437.74	K	Joback Method
vc	1.026	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	825.38	J/mol×K	756.46	Joback Method
cpg	842.73	J/mol×K	788.16	Joback Method
cpg	859.04	J/mol×K	819.86	Joback Method
cpg	874.34	J/mol×K	851.56	Joback Method
cpg	888.66	J/mol×K	883.25	Joback Method
cpg	902.02	J/mol×K	914.95	Joback Method
cpg	914.46	J/mol×K	946.65	Joback Method
dvisc	0.0008966	Pa×s	437.74	Joback Method

dvisc	0.0003976	Pa×s	490.86	Joback Method
dvisc	0.0002067	Pa×s	543.98	Joback Method
dvisc	0.0001207	Pa×s	597.10	Joback Method
dvisc	0.0000770	Pa×s	650.22	Joback Method
dvisc	0.0000525	Pa×s	703.34	Joback Method
dvisc	0.0000378	Pa×s	756.46	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=U368395&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