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

Inchi: InChI=1S/C16H30O5/c1-8-16(9-2,13(17)19-10-3)14(18)21-12(4)11-20-15(5,6)7/h12H,8-1

InchiKey: TWOPSTSLOZAQRH-UHFFFAOYSA-N

Formula: C16H30O5

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

Mol. weight [g/mol]: 302.41

Physical Properties

Property code	Value	Unit	Source
gf	-485.76	kJ/mol	Joback Method
hf	-1018.17	kJ/mol	Joback Method
hfus	25.61	kJ/mol	Joback Method
hvap	68.95	kJ/mol	Joback Method
log10ws	-3.31		Crippen Method
logp	3.103		Crippen Method
mcvol	257.050	ml/mol	McGowan Method
pc	1442.44	kPa	Joback Method
rinpol	1645.00		NIST Webbook
rinpol	1645.00		NIST Webbook
tb	733.58	K	Joback Method
tc	924.25	K	Joback Method
tf	426.47	K	Joback Method
vc	0.970	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	767.98	J/mol×K	733.58	Joback Method
cpg	785.09	J/mol×K	765.36	Joback Method
cpg	801.18	J/mol×K	797.14	Joback Method
cpg	816.28	J/mol×K	828.92	Joback Method
cpg	830.42	J/mol×K	860.69	Joback Method
cpg	843.64	J/mol×K	892.47	Joback Method
cpg	855.95	J/mol×K	924.25	Joback Method
dvisc	0.0010225	Pa×s	426.47	Joback Method

dvisc	0.0004582	Pa×s	477.66	Joback Method
dvisc	0.0002398	Pa×s	528.84	Joback Method
dvisc	0.0001407	Pa×s	580.02	Joback Method
dvisc	0.0000900	Pa×s	631.21	Joback Method
dvisc	0.0000616	Pa×s	682.39	Joback Method
dvisc	0.0000444	Pa×s	733.58	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U368394&Units=SI
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

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