Diethylmalonic acid, di(1-tert-butyloxyprop-2-yl) ester

Inchi: InChI=1S/C21H40O6/c1-11-21(12-2,17(22)26-15(3)13-24-19(5,6)7)18(23)27-16(4)14-25-
InchiKey: VRGDRQIILBDECD-UHFFFAOYSA-N
Formula: C21H40O6
SMILES: CCC(CC)(C(=O)OC(C)COC(C)(C)C)C(=O)OC(C)COC(C)(C)C
Mol. weight [g/mol]: 388.54

Physical Properties

Property code	Value	Unit	Source
gf	-548.26	kJ/mol	Joback Method
hf	-1267.62	kJ/mol	Joback Method
hfus	28.81	kJ/mol	Joback Method
hvap	80.81	kJ/mol	Joback Method
log10ws	-4.72		Crippen Method
logp	4.286		Crippen Method
mcvol	333.370	ml/mol	McGowan Method
pc	1038.57	kPa	Joback Method
rinpol	1993.00		NIST Webbook
rinpol	1993.00		NIST Webbook
tb	866.73	K	Joback Method
tc	1067.49	K	Joback Method
tf	492.47	K	Joback Method
vc	1.250	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1096.06	J/mol×K	866.73	Joback Method
cpg	1114.05	J/mol×K	900.19	Joback Method
cpg	1130.75	J/mol×K	933.65	Joback Method
cpg	1146.22	J/mol×K	967.11	Joback Method
cpg	1160.49	J/mol×K	1000.57	Joback Method
cpg	1173.61	J/mol×K	1034.03	Joback Method
cpg	1185.65	J/mol×K	1067.49	Joback Method
dvisc	0.0003639	Pa×s	492.47	Joback Method

dvisc	0.0001438	Pa×s	554.85	Joback Method
dvisc	0.0000686	Pa×s	617.22	Joback Method
dvisc	0.0000375	Pa×s	679.60	Joback Method
dvisc	0.0000227	Pa×s	741.98	Joback Method
dvisc	0.0000148	Pa×s	804.35	Joback Method
dvisc	0.0000103	Pa×s	866.73	Joback Method

Sources

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=U368397&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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