Dimethylmalonic acid, di(2-ethylphenyl) ester

Inchi: InChI=1S/C21H24O4/c1-5-15-11-7-9-13-17(15)24-19(22)21(3,4)20(23)25-18-14-10-8-12-
InchiKey: ZQNPYCFHSBNJAL-UHFFFAOYSA-N
Formula: C21H24O4
SMILES: CCc1ccccc1OC(=O)C(C)(C)C(=O)Oc1ccccc1CC
Mol. weight [g/mol]: 340.41

Physical Properties

Property code	Value	Unit	Source
gf	-133.50	kJ/mol	Joback Method
hf	-525.00	kJ/mol	Joback Method
hfus	35.61	kJ/mol	Joback Method
hvap	85.23	kJ/mol	Joback Method
log10ws	-5.53		Crippen Method
logp	4.349		Crippen Method
mcvol	274.110	ml/mol	McGowan Method
pc	1611.58	kPa	Joback Method
rinpol	2362.00		NIST Webbook
tb	892.55	K	Joback Method
tc	1123.35	K	Joback Method
tf	551.05	K	Joback Method
vc	1.032	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	839.04	J/mol×K	892.55	Joback Method
cpg	853.47	J/mol×K	931.02	Joback Method
cpg	866.60	J/mol×K	969.48	Joback Method
cpg	878.46	J/mol×K	1007.95	Joback Method
cpg	889.14	J/mol×K	1046.41	Joback Method
cpg	898.69	J/mol×K	1084.88	Joback Method
cpg	907.17	J/mol×K	1123.35	Joback Method
dvisc	0.0003639	Pa×s	551.05	Joback Method
dvisc	0.0002102	Pa×s	607.97	Joback Method

dvisc	0.0001334	Pa×s	664.88	Joback Method
dvisc	0.0000910	Pa×s	721.80	Joback Method
dvisc	0.0000656	Pa×s	778.72	Joback Method
dvisc	0.0000495	Pa×s	835.63	Joback Method
dvisc	0.0000387	Pa×s	892.55	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=U363853&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