Dimethylmalonic acid, ethyl 2-methylphenyl ester

Inchi: InChI=1S/C14H18O4/c1-5-17-12(15)14(3,4)13(16)18-11-9-7-6-8-10(11)2/h6-9H,5H2,1-4

InchiKey: ZALSQJZHOKEFPD-UHFFFAOYSA-N

Formula: C14H18O4

SMILES: CCOC(=O)C(C)(C)C(=O)Oc1ccccc1C

Mol. weight [g/mol]: 250.29

Physical Properties

Property code	Value	Unit	Source
gf	-295.22	kJ/mol	Joback Method
hf	-605.58	kJ/mol	Joback Method
hfus	23.83	kJ/mol	Joback Method
hvap	66.71	kJ/mol	Joback Method
log10ws	-2.97		Crippen Method
logp	2.490		Crippen Method
mcvol	199.240	ml/mol	McGowan Method
pc	2193.84	kPa	Joback Method
rinpol	1629.00		NIST Webbook
rinpol	1629.00		NIST Webbook
tb	700.73	K	Joback Method
tc	917.02	K	Joback Method
tf	433.22	K	Joback Method
vc	0.749	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	542.67	J/mol×K	700.73	Joback Method
cpg	606.83	J/mol×K	880.97	Joback Method
cpg	595.93	J/mol×K	844.93	Joback Method
cpg	584.09	J/mol×K	808.88	Joback Method
cpg	571.28	J/mol×K	772.83	Joback Method
cpg	557.49	J/mol×K	736.78	Joback Method
cpg	616.83	J/mol×K	917.02	Joback Method
dvisc	0.0001000	Pa×s	700.73	Joback Method

dvisc	0.0001285	Pa×s	656.14	Joback Method
dvisc	0.0001714	Pa×s	611.56	Joback Method
dvisc	0.0002390	Pa×s	566.98	Joback Method
dvisc	0.0003529	Pa×s	522.39	Joback Method
dvisc	0.0005603	Pa×s	477.81	Joback Method
dvisc	0.0009784	Pa×s	433.22	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=U361911&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