Dimethylmalonic acid, diphenyl ester

Inchi: InChI=1S/C17H16O4/c1-17(2,15(18)20-13-9-5-3-6-10-13)16(19)21-14-11-7-4-8-12-14/h3
InchiKey: HWZVGGMEXHEECA-UHFFFAOYSA-N
Formula: C17H16O4
SMILES: CC(C)(C(=O)Oc1ccccc1)C(=O)Oc1ccccc1
Mol. weight [g/mol]: 284.31
CAS: 26595-27-7

Physical Properties

Property code	Value	Unit	Source
gf	-147.92	kJ/mol	Joback Method
hf	-419.50	kJ/mol	Joback Method
hfus	26.03	kJ/mol	Joback Method
hvap	75.00	kJ/mol	Joback Method
log10ws	-3.92		Crippen Method
logp	3.224		Crippen Method
mcvol	217.750	ml/mol	McGowan Method
pc	2318.07	kPa	Joback Method
rinpol	2028.00		NIST Webbook
tb	791.07	K	Joback Method
tc	1033.95	K	Joback Method
tf	480.93	K	Joback Method
vc	0.808	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	616.05	J/mol×K	791.07	Joback Method
cpg	630.27	J/mol×K	831.55	Joback Method
cpg	643.15	J/mol×K	872.03	Joback Method
cpg	654.75	J/mol×K	912.51	Joback Method
cpg	665.15	J/mol×K	952.99	Joback Method
cpg	674.43	J/mol×K	993.47	Joback Method
cpg	682.66	J/mol×K	1033.95	Joback Method
dvisc	0.0007418	Pa×s	480.93	Joback Method

dvisc	0.0004086	Pa×s	532.62	Joback Method
dvisc	0.0002501	Pa×s	584.31	Joback Method
dvisc	0.0001658	Pa×s	636.00	Joback Method
dvisc	0.0001169	Pa×s	687.69	Joback Method
dvisc	0.0000866	Pa×s	739.38	Joback Method
dvisc	0.0000667	Pa×s	791.07	Joback Method

Sources

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=C26595277&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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