Dimethylmalonic acid, di(2-phenethyl) ester

Inchi: InChI=1S/C21H24O4/c1-21(2,19(22)24-15-13-17-9-5-3-6-10-17)20(23)25-16-14-18-11-7-
InchiKey: SKBRKUZQKUIQNK-UHFFFAOYSA-N
Formula: C21H24O4
SMILES: CC(C)(C(=O)OCCc1ccccc1)C(=O)OCCc1ccccc1
Mol. weight [g/mol]: 340.41

Physical Properties

Property code	Value	Unit	Source
gf	-114.24	kJ/mol	Joback Method
hf	-502.06	kJ/mol	Joback Method
hfus	36.39	kJ/mol	Joback Method
hvap	83.91	kJ/mol	Joback Method
log10ws	-4.30		Crippen Method
logp	3.584		Crippen Method
mcvol	274.110	ml/mol	McGowan Method
pc	1651.11	kPa	Joback Method
rinpol	2445.00		NIST Webbook
rinpol	2445.00		NIST Webbook
tb	882.59	K	Joback Method
tc	1111.91	K	Joback Method
tf	526.01	K	Joback Method
vc	1.032	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	841.26	J/mol×K	882.59	Joback Method
cpg	855.91	J/mol×K	920.81	Joback Method
cpg	869.25	J/mol×K	959.03	Joback Method
cpg	881.37	J/mol×K	997.25	Joback Method
cpg	892.33	J/mol×K	1035.47	Joback Method
cpg	902.22	J/mol×K	1073.69	Joback Method
cpg	911.12	J/mol×K	1111.91	Joback Method
dvisc	0.0004843	Pa×s	526.01	Joback Method

dvisc	0.0002546	Pa×s	585.44	Joback Method
dvisc	0.0001507	Pa×s	644.87	Joback Method
dvisc	0.0000974	Pa×s	704.30	Joback Method
dvisc	0.0000674	Pa×s	763.73	Joback Method
dvisc	0.0000492	Pa×s	823.16	Joback Method
dvisc	0.0000375	Pa×s	882.59	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=U361629&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