Dimethylmalonic acid, isobutyl 3-phenylpropyl ester

Inchi: InChI=1S/C18H26O4/c1-14(2)13-22-17(20)18(3,4)16(19)21-12-8-11-15-9-6-5-7-10-15/h5

InchiKey: NPJMRBUJLXYPCU-UHFFFAOYSA-N

Formula: C18H26O4

SMILES: CC(C)COC(=O)C(C)(C)C(=O)OCCCc1ccccc1

Mol. weight [g/mol]: 306.40

Physical Properties

Property code	Value	Unit	Source
gf	-254.35	kJ/mol	Joback Method
hf	-681.95	kJ/mol	Joback Method
hfus	31.05	kJ/mol	Joback Method
hvap	74.57	kJ/mol	Joback Method
log10ws	-3.70		Crippen Method
logp	3.388		Crippen Method
mcvol	255.600	ml/mol	McGowan Method
pc	1605.13	kPa	Joback Method
rinpol	2001.00		NIST Webbook
rinpol	2001.00		NIST Webbook
tb	786.83	K	Joback Method
tc	995.48	K	Joback Method
tf	450.78	K	Joback Method
vc	0.967	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	764.08	J/mol×K	786.83	Joback Method
cpg	834.23	J/mol×K	960.71	Joback Method
cpg	822.33	J/mol×K	925.93	Joback Method
cpg	809.42	J/mol×K	891.16	Joback Method
cpg	795.43	J/mol×K	856.38	Joback Method
cpg	780.34	J/mol×K	821.61	Joback Method
cpg	845.14	J/mol×K	995.48	Joback Method
dvisc	0.0000531	Pa×s	786.83	Joback Method

dvisc	0.0000714	Pa×s	730.82	Joback Method
dvisc	0.0001010	Pa×s	674.81	Joback Method
dvisc	0.0001522	Pa×s	618.81	Joback Method
dvisc	0.0002487	Pa×s	562.80	Joback Method
dvisc	0.0004530	Pa×s	506.79	Joback Method
dvisc	0.0009577	Pa×s	450.78	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=U361831&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