Dimethylmalonic acid, 3-phenylpropyl propyl ester

Inchi: InChI=1S/C17H24O4/c1-4-12-20-15(18)17(2,3)16(19)21-13-8-11-14-9-6-5-7-10-14/h5-7,

InchiKey: DEZPNESOACKNSA-UHFFFAOYSA-N

Formula: C17H24O4

SMILES: CCCOC(=O)C(C)(C)C(=O)OCCCc1ccccc1

Mol. weight [g/mol]: 292.37

Physical Properties

Property code	Value	Unit	Source
gf	-260.33	kJ/mol	Joback Method
hf	-656.03	kJ/mol	Joback Method
hfus	31.99	kJ/mol	Joback Method
hvap	72.73	kJ/mol	Joback Method
log10ws	-3.53		Crippen Method
logp	3.142		Crippen Method
mcvol	241.510	ml/mol	McGowan Method
pc	1724.59	kPa	Joback Method
rinpol	1950.00		NIST Webbook
tb	764.39	K	Joback Method
tc	971.89	K	Joback Method
tf	454.51	K	Joback Method
vc	0.916	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	706.97	J/mol×K	764.39	Joback Method
cpg	722.81	J/mol×K	798.97	Joback Method
cpg	737.54	J/mol×K	833.56	Joback Method
cpg	751.22	J/mol×K	868.14	Joback Method
cpg	763.87	J/mol×K	902.73	Joback Method
cpg	775.55	J/mol×K	937.31	Joback Method
cpg	786.29	J/mol×K	971.89	Joback Method
dvisc	0.0009021	Pa×s	454.51	Joback Method
dvisc	0.0004682	Pa×s	506.16	Joback Method

dvisc	0.0002743	Pa×s	557.80	Joback Method
dvisc	0.0001760	Pa×s	609.45	Joback Method
dvisc	0.0001210	Pa×s	661.10	Joback Method
dvisc	0.0000879	Pa×s	712.74	Joback Method
dvisc	0.0000666	Pa×s	764.39	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=U361830&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