Dimethylmalonic acid, ethyl 3-phenylpropyl ester

Inchi: InChI=1S/C16H22O4/c1-4-19-14(17)16(2,3)15(18)20-12-8-11-13-9-6-5-7-10-13/h5-7,9-1

InchiKey: UVZGDZMWSQFVEJ-UHFFFAOYSA-N

Formula: C16H22O4

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

Mol. weight [g/mol]: 278.34

Physical Properties

Property code	Value	Unit	Source
gf	-268.75	kJ/mol	Joback Method
hf	-635.39	kJ/mol	Joback Method
hfus	29.40	kJ/mol	Joback Method
hvap	70.50	kJ/mol	Joback Method
log10ws	-3.11		Crippen Method
logp	2.752		Crippen Method
mcvol	227.420	ml/mol	McGowan Method
pc	1870.79	kPa	Joback Method
rinpol	1858.00		NIST Webbook
tb	741.51	K	Joback Method
tc	951.19	K	Joback Method
tf	443.24	K	Joback Method
vc	0.861	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	651.40	J/mol×K	741.51	Joback Method
cpg	667.00	J/mol×K	776.46	Joback Method
cpg	681.51	J/mol×K	811.40	Joback Method
cpg	694.98	J/mol×K	846.35	Joback Method
cpg	707.44	J/mol×K	881.30	Joback Method
cpg	718.93	J/mol×K	916.25	Joback Method
cpg	729.50	J/mol×K	951.19	Joback Method
dvisc	0.0009978	Pa×s	443.24	Joback Method
dvisc	0.0005244	Pa×s	492.95	Joback Method

dvisc	0.0003101	Pa×s	542.66	Joback Method
dvisc	0.0002003	Pa×s	592.38	Joback Method
dvisc	0.0001384	Pa×s	642.09	Joback Method
dvisc	0.0001008	Pa×s	691.80	Joback Method
dvisc	0.0000767	Pa×s	741.51	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U361829&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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

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