

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/h5-7,9-11
InchiKey:	UVZGDZMWSQFVEJ-UHFFFAOYSA-N
Formula:	C16H22O4
SMILES:	CCOC(=O)C(C)(C)C(=O)OCCc1ccccc1
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	m ³ /kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0003101	Paxs	542.66	Joback Method
dvisc	0.0002003	Paxs	592.38	Joback Method
dvisc	0.0001384	Paxs	642.09	Joback Method
dvisc	0.0001008	Paxs	691.80	Joback Method
dvisc	0.0000767	Paxs	741.51	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U361829&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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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