

Dimethylmalonic acid, ethyl phenyl ester

Inchi:	InChI=1S/C13H16O4/c1-4-16-11(14)13(2,3)12(15)17-10-8-6-5-7-9-10/h5-9H,4H2,1-3H3
InchiKey:	BAIWHDLHWMYSAJ-UHFFFAOYSA-N
Formula:	C13H16O4
SMILES:	CCOC(=O)C(C)(C)C(=O)Oc1ccccc1
Mol. weight [g/mol]:	236.26

Physical Properties

Property code	Value	Unit	Source
gf	-294.01	kJ/mol	Joback Method
hf	-573.47	kJ/mol	Joback Method
hfus	21.63	kJ/mol	Joback Method
hvap	63.82	kJ/mol	Joback Method
log10ws	-2.50		Crippen Method
logp	2.181		Crippen Method
mcvol	185.150	ml/mol	McGowan Method
pc	2441.06	kPa	Joback Method
rinpol	1539.00		NIST Webbook
rinpol	1539.00		NIST Webbook
tb	672.87	K	Joback Method
tc	891.86	K	Joback Method
tf	409.43	K	Joback Method
vc	0.693	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	491.44	J/molxK	672.87	Joback Method
cpg	506.01	J/molxK	709.37	Joback Method
cpg	519.54	J/molxK	745.87	Joback Method
cpg	532.08	J/molxK	782.37	Joback Method
cpg	543.65	J/molxK	818.86	Joback Method
cpg	554.30	J/molxK	855.36	Joback Method
cpg	564.05	J/molxK	891.86	Joback Method
dvisc	0.0013071	Paxs	409.43	Joback Method

dvisc	0.0007159	Paxs	453.34	Joback Method
dvisc	0.0004361	Paxs	497.24	Joback Method
dvisc	0.0002879	Paxs	541.15	Joback Method
dvisc	0.0002023	Paxs	585.06	Joback Method
dvisc	0.0001493	Paxs	628.96	Joback Method
dvisc	0.0001146	Paxs	672.87	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U361806&Units=SI

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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