Malonamic acid, 2-ethyl-2-phenyl-, methyl ester

Inchi: InChI=1S/C12H15NO3/c1-3-12(10(13)14,11(15)16-2)9-7-5-4-6-8-9/h4-8H,3H2,1-2H3,(H2

InchiKey: PPRJPTXCOUBNPG-UHFFFAOYSA-N

Formula: C12H15NO3

SMILES: CCC(C(=N)O)(C(=O)OC)c1ccccc1

Mol. weight [g/mol]: 221.25

CAS: 19846-01-6

Physical Properties

Property code	Value	Unit	Source
gf	-1.73	kJ/mol	Joback Method
hf	-261.93	kJ/mol	Joback Method
hvap	81.20	kJ/mol	Joback Method
log10ws	-3.22		Crippen Method
logp	2.043		Crippen Method
mcvol	175.170	ml/mol	McGowan Method
tb	750.22	K	Joback Method
tf	455.60	K	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	493.39	J/mol×K	750.22	Joback Method
cpg	66.28	J/mol×K	100.12	Joback Method
cpg	66.28	J/mol×K	100.12	Joback Method
cpg	66.28	J/mol×K	100.12	Joback Method
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cpg	66.28	J/mol×K	100.12	Joback Method
cpg	66.28	J/mol×K	100.12	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=C19846016&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation 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
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point