Propanedioic acid, (phenylmethylene)-, diethyl ester

Other names: Malonic acid, benzylidene-, diethyl ester
Benzylidenemalonic acid diethyl ester
Diethyl benzalmalonate
Diethyl benzylidenemalonate
Ethyl benzylidenemalonate
«beta»,«beta»-Diethoxycarbonylstyrene
Diethyl (phenylmethylene)malonate
2-Benzylidene-malonic acid diethyl ester

Inchi: InChI=1S/C14H16O4/c1-3-17-13(15)12(14(16)18-4-2)10-11-8-6-5-7-9-11/h5-10H,3-4H2,

InchiKey: VUWPIBNKJSEYIN-UHFFFAOYSA-N

Formula: C14H16O4

SMILES: CCOC(=O)C(=Cc1ccccc1)C(=O)OCC

Mol. weight [g/mol]: 248.27

CAS: 5292-53-5

Physical Properties

Property code	Value	Unit	Source
gf	-216.76	kJ/mol	Joback Method
hf	-477.93	kJ/mol	Joback Method
hfus	30.52	kJ/mol	Joback Method
hvap	67.38	kJ/mol	Joback Method
log10ws	-2.53		Crippen Method
logp	2.196		Crippen Method
mcvol	194.940	ml/mol	McGowan Method
pc	2306.95	kPa	Joback Method
tb	703.02	K	Joback Method
tc	918.65	K	Joback Method
tf	399.24	K	Joback Method
vc	0.741	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	517.28	J/mol×K	703.02	Joback Method

cpg	531.41	J/mol×K	738.96	Joback Method
cpg	544.59	J/mol×K	774.90	Joback Method
cpg	556.84	J/mol×K	810.83	Joback Method
cpg	568.20	J/mol×K	846.77	Joback Method
cpg	578.70	J/mol×K	882.71	Joback Method
cpg	588.35	J/mol×K	918.65	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	489.20	K	4.00	NIST Webbook
tbrp	469.20	K	1.90	NIST Webbook

Sources

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=C5292535&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg: Ideal gas heat capacity
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
tb: Normal Boiling Point Temperature
tbrp: Boiling point at reduced pressure
tc: Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume

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