Propanedioic acid, phenyl-, diethyl ester

Other names: Malonic acid, phenyl-, diethyl ester
Diethyl phenylmalonate
Phenylmalonic acid diethyl ester
Inchi: InChI=1S/C13H16O4/c1-3-16-12(14)11(13(15)17-4-2)10-8-6-5-7-9-10/h5-9,11H,3-4H2,1-
InchiKey: FGYDHYCFHBSNPE-UHFFFAOYSA-N
Formula: C13H16O4
SMILES: CCOC(=O)C(C(=O)OCC)c1ccccc1
Mol. weight [g/mol]: 236.26
CAS: 83-13-6

Physical Properties

Property code	Value	Unit	Source
gf	-299.29	kJ/mol	Joback Method
hf	-570.00	kJ/mol	Joback Method
hfus	25.52	kJ/mol	Joback Method
hvap	64.73	kJ/mol	Joback Method
log10ws	-2.06		Crippen Method
logp	1.896		Crippen Method
mcvol	185.150	ml/mol	McGowan Method
pc	2414.74	kPa	Joback Method
tb	675.66	K	Joback Method
tc	887.29	K	Joback Method
tf	392.01	K	Joback Method
vc	0.698	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	489.00	J/mol×K	675.66	Joback Method
cpg	503.34	J/mol×K	710.93	Joback Method
cpg	516.76	J/mol×K	746.20	Joback Method
cpg	529.27	J/mol×K	781.48	Joback Method
cpg	540.88	J/mol×K	816.75	Joback Method
cpg	551.59	J/mol×K	852.02	Joback Method

cpg	561.42	J/mol×K	887.29	Joback Method
dvisc	0.0015325	Pa×s	392.01	Joback Method
dvisc	0.0008056	Pa×s	439.29	Joback Method
dvisc	0.0004799	Pa×s	486.56	Joback Method
dvisc	0.0003133	Pa×s	533.84	Joback Method
dvisc	0.0002193	Pa×s	581.11	Joback Method
dvisc	0.0001619	Pa×s	628.38	Joback Method
dvisc	0.0001247	Pa×s	675.66	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	444.20	K	1.90	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C83136&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
tb: Normal Boiling Point Temperature

tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume