Propanedioic acid, (phenylmethyl)-, diethyl ester

Other names: Diethyl benzylmalonate
Benzylmalonic acid diethyl ester
Malonic acid, benzyl-, diethyl ester
Malonic acid, 2-benzyl-, diethyl ester

Inchi: InChI=1S/C14H18O4/c1-3-17-13(15)12(14(16)18-4-2)10-11-8-6-5-7-9-11/h5-9,12H,3-4,1

InchiKey: ICZLTZWATFXDLP-UHFFFAOYSA-N

Formula: C14H18O4

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

Mol. weight [g/mol]: 250.29

CAS: 607-81-8

Physical Properties

Property code	Value	Unit	Source
gf	-290.87	kJ/mol	Joback Method
hf	-590.64	kJ/mol	Joback Method
hfus	28.11	kJ/mol	Joback Method
hvap	66.96	kJ/mol	Joback Method
log10ws	-2.27		Crippen Method
logp	1.971		Crippen Method
mcvol	199.240	ml/mol	McGowan Method
pc	2202.08	kPa	Joback Method
tb	573.20	K	NIST Webbook
tc	907.17	K	Joback Method
tf	403.28	K	Joback Method
vc	0.753	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	541.37	J/mol×K	698.54	Joback Method
cpg	605.85	J/mol×K	872.40	Joback Method
cpg	594.82	J/mol×K	837.63	Joback Method
cpg	582.87	J/mol×K	802.86	Joback Method
cpg	569.99	J/mol×K	768.08	Joback Method

cpg	556.16	J/mol×K	733.31	Joback Method
cpg	615.97	J/mol×K	907.17	Joback Method
dvisc	0.0001106	Pa×s	698.54	Joback Method
dvisc	0.0001441	Pa×s	649.33	Joback Method
dvisc	0.0001960	Pa×s	600.12	Joback Method
dvisc	0.0002817	Pa×s	550.91	Joback Method
dvisc	0.0004347	Pa×s	501.70	Joback Method
dvisc	0.0007371	Pa×s	452.49	Joback Method
dvisc	0.0014220	Pa×s	403.28	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	435.70	K	1.30	NIST Webbook
tbrp	442.20	K	1.60	NIST Webbook

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=C607818&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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