Benzeneacetic acid, «alpha»-phenyl-, methyl ester

Other names: Acetic acid, diphenyl-, methyl ester
Diphenylacetic acid, methyl ester
Methyl diphenylacetate

Inchi: InChI=1S/C15H14O2/c1-17-15(16)14(12-8-4-2-5-9-12)13-10-6-3-7-11-13/h2-11,14H,1H3

InchiKey: AORIUCNKPVHMTN-UHFFFAOYSA-N

Formula: C15H14O2

SMILES: COC(=O)C(c1ccccc1)c1ccccc1

Mol. weight [g/mol]: 226.27

CAS: 3469-00-9

Physical Properties

Property code	Value	Unit	Source
gf	63.88	kJ/mol	Joback Method
hf	-129.95	kJ/mol	Joback Method
hfus	21.95	kJ/mol	Joback Method
hvap	62.30	kJ/mol	Joback Method
log10ws	-3.24		Crippen Method
logp	2.991		Crippen Method
mcvol	182.130	ml/mol	McGowan Method
pc	2651.56	kPa	Joback Method
rinpol	1740.00		NIST Webbook
rinpol	1775.00		NIST Webbook
tb	671.81	K	Joback Method
tc	914.44	K	Joback Method
tf	368.81	K	Joback Method
vc	0.677	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	467.27	J/mol×K	671.81	Joback Method
cpg	535.55	J/mol×K	874.00	Joback Method
cpg	524.26	J/mol×K	833.56	Joback Method
cpg	511.85	J/mol×K	793.13	Joback Method

cpg	498.25	J/mol×K	752.69	Joback Method
cpg	483.41	J/mol×K	712.25	Joback Method
cpg	545.78	J/mol×K	914.44	Joback Method
dvisc	0.0001264	Pa×s	671.81	Joback Method
dvisc	0.0001649	Pa×s	621.31	Joback Method
dvisc	0.0002254	Pa×s	570.81	Joback Method
dvisc	0.0003275	Pa×s	520.31	Joback Method
dvisc	0.0005154	Pa×s	469.81	Joback Method
dvisc	0.0009050	Pa×s	419.31	Joback Method
dvisc	0.0018537	Pa×s	368.81	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C3469009&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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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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