Propanoic acid, 2-phenoxy-, methyl ester

Other names: Methyl 2-phenoxypropionate
Inchi: InChI=1S/C10H12O3/c1-8(10(11)12-2)13-9-6-4-3-5-7-9/h3-8H,1-2H3
InchiKey: KIBRBMKSBVQDMK-UHFFFAOYSA-N
Formula: C10H12O3
SMILES: COC(=O)C(C)Oc1ccccc1
Mol. weight [g/mol]: 180.20
CAS: 2065-24-9

Physical Properties

Property code	Value	Unit	Source
gf	-195.63	kJ/mol	Joback Method
hf	-395.50	kJ/mol	Joback Method
hfus	16.15	kJ/mol	Joback Method
hvap	51.31	kJ/mol	Joback Method
log10ws	-1.82		Crippen Method
logp	1.627		Crippen Method
mcvol	141.310	ml/mol	McGowan Method
pc	3052.41	kPa	Joback Method
rinpol	1258.00		NIST Webbook
tb	553.15	K	Joback Method
tc	768.17	K	Joback Method
tf	308.27	K	Joback Method
vc	0.523	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	324.75	J/mol×K	553.15	Joback Method
cpg	338.43	J/mol×K	588.99	Joback Method
cpg	351.37	J/mol×K	624.82	Joback Method
cpg	363.58	J/mol×K	660.66	Joback Method
cpg	375.04	J/mol×K	696.50	Joback Method
cpg	385.78	J/mol×K	732.34	Joback Method
cpg	395.79	J/mol×K	768.17	Joback Method

dvisc	0.0022528	Pa×s	308.27	Joback Method
dvisc	0.0011324	Pa×s	349.08	Joback Method
dvisc	0.0006573	Pa×s	389.90	Joback Method
dvisc	0.0004230	Pa×s	430.71	Joback Method
dvisc	0.0002938	Pa×s	471.52	Joback Method
dvisc	0.0002163	Pa×s	512.34	Joback Method
dvisc	0.0001666	Pa×s	553.15	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2065249&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume