Acetic acid, phenoxy-, methyl ester

Other names:	Methyl phenoxyacetate
	Phenoxyacetic acid methyl ester
Inchi:	InChI=1S/C9H10O3/c1-11-9(10)7-12-8-5-3-2-4-6-8/h2-6H,7H2,1H3
InchiKey:	BZCKRPHEZOHHBK-UHFFFAOYSA-N
Formula:	C9H10O3
SMILES:	COC(=O)COc1ccccc1
Mol. weight [g/mol]:	166.17
CAS:	2065-23-8

Physical Properties

Property code	Value	Unit	Source
gf	-201.61	kJ/mol	Joback Method
hf	-369.58	kJ/mol	Joback Method
hfus	17.08	kJ/mol	Joback Method
hvap	49.47	kJ/mol	Joback Method
log10ws	-1.29		Crippen Method
logp	1.238		Crippen Method
mcvol	127.220	ml/mol	McGowan Method
pc	3372.36	kPa	Joback Method
rinpol	221.90		NIST Webbook
rinpol	1271.00		NIST Webbook
rinpol	1271.00		NIST Webbook
rinpol	221.90		NIST Webbook
rinpol	1260.00		NIST Webbook
tb	518.20	K	NIST Webbook
tb	516.20	K	NIST Webbook
tc	744.61	K	Joback Method
tf	312.00	K	Joback Method
vc	0.473	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	279.36	J/mol×K	530.71	Joback Method

cpg	291.72	J/mol×K	566.36	Joback Method
cpg	303.45	J/mol×K	602.01	Joback Method
cpg	314.53	J/mol×K	637.66	Joback Method
cpg	324.98	J/mol×K	673.31	Joback Method
cpg	334.79	J/mol×K	708.96	Joback Method
cpg	343.96	J/mol×K	744.61	Joback Method
dvisc	0.0017696	Pa×s	312.00	Joback Method
dvisc	0.0010069	Pa×s	348.45	Joback Method
dvisc	0.0006375	Pa×s	384.90	Joback Method
dvisc	0.0004369	Pa×s	421.36	Joback Method
dvisc	0.0003179	Pa×s	457.81	Joback Method
dvisc	0.0002425	Pa×s	494.26	Joback Method
dvisc	0.0001920	Pa×s	530.71	Joback Method

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2065238&Units=SI

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