1-Phenoxypropan-2-yl acetate

Other names: Phenoxyisopropanyl acetate
2-Phenoxy-1-methylethyl acetate
Inchi: InChI=1S/C11H14O3/c1-9(14-10(2)12)8-13-11-6-4-3-5-7-11/h3-7,9H,8H2,1-2H3
InchiKey: QWWTXMUURQLKOT-UHFFFAOYSA-N
Formula: C11H14O3
SMILES: CC(=O)OC(C)COc1ccccc1
Mol. weight [g/mol]: 194.23

Physical Properties

Property code	Value	Unit	Source
gf	-187.21	kJ/mol	Joback Method
hf	-416.14	kJ/mol	Joback Method
hfus	18.74	kJ/mol	Joback Method
hvap	53.53	kJ/mol	Joback Method
log10ws	-2.24		Crippen Method
logp	2.017		Crippen Method
mcvol	155.400	ml/mol	McGowan Method
pc	2752.67	kPa	Joback Method
rinpol	1436.00		NIST Webbook
tb	576.03	K	Joback Method
tc	787.48	K	Joback Method
tf	319.54	K	Joback Method
vc	0.580	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	371.61	J/mol×K	576.03	Joback Method
cpg	436.27	J/mol×K	752.24	Joback Method
cpg	424.90	J/mol×K	717.00	Joback Method
cpg	412.76	J/mol×K	681.76	Joback Method
cpg	399.83	J/mol×K	646.51	Joback Method
cpg	386.12	J/mol×K	611.27	Joback Method
cpg	446.86	J/mol×K	787.48	Joback Method

dvisc	0.0001521	Pa×s	576.03	Joback Method
dvisc	0.0001984	Pa×s	533.28	Joback Method
dvisc	0.0002709	Pa×s	490.53	Joback Method
dvisc	0.0003927	Pa×s	447.78	Joback Method
dvisc	0.0006157	Pa×s	405.04	Joback Method
dvisc	0.0010734	Pa×s	362.29	Joback Method
dvisc	0.0021712	Pa×s	319.54	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U372958&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