Benzenemethanol, 3-phenoxy-, acetate

Other names: Acetic acid, (3-phenoxyphenyl)methyl ester
m-phenoxybenzyl acetate
Inchi: InChI=1S/C15H14O3/c1-12(16)17-11-13-6-5-9-15(10-13)18-14-7-3-2-4-8-14/h2-10H,11H
InchiKey: XPHQNMNGUGOWGU-UHFFFAOYSA-N
Formula: C15H14O3
SMILES: CC(=O)OCc1cccc(Oc2ccccc2)c1
Mol. weight [g/mol]: 242.27
CAS: 50789-44-1

Physical Properties

Property code	Value	Unit	Source
gf	-48.31	kJ/mol	Joback Method
hf	-268.36	kJ/mol	Joback Method
hfus	26.27	kJ/mol	Joback Method
hvap	65.76	kJ/mol	Joback Method
log10ws	-3.69		Crippen Method
logp	3.542		Crippen Method
mcvol	188.000	ml/mol	McGowan Method
pc	2545.61	kPa	Joback Method
rinpol	1918.00		NIST Webbook
rinpol	1918.00		NIST Webbook
tb	699.65	K	Joback Method
tc	934.64	K	Joback Method
tf	418.56	K	Joback Method
vc	0.702	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	491.63	J/mol×K	699.65	Joback Method
cpg	506.76	J/mol×K	738.81	Joback Method
cpg	520.73	J/mol×K	777.98	Joback Method
cpg	533.56	J/mol×K	817.14	Joback Method
cpg	545.27	J/mol×K	856.31	Joback Method

cpg	555.89	J/mol×K	895.47	Joback Method
cpg	565.45	J/mol×K	934.64	Joback Method
dvisc	0.0009037	Pa×s	418.56	Joback Method
dvisc	0.0005287	Pa×s	465.41	Joback Method
dvisc	0.0003412	Pa×s	512.26	Joback Method
dvisc	0.0002370	Pa×s	559.11	Joback Method
dvisc	0.0001741	Pa×s	605.95	Joback Method
dvisc	0.0001337	Pa×s	652.80	Joback Method
dvisc	0.0001064	Pa×s	699.65	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C50789441&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