2-Phenoxyethyl isobutyrate

Other names:	Propanoic acid, 2-methyl-, 2-phenoxyethyl ester
	Isobutyric acid, 2-phenoxyethyl ester
	«beta»-Phenoxyethyl iso-butyrate
	Phenoxyethyl isobutyrate
Inchi:	InChI=1S/C12H16O3/c1-10(2)12(13)15-9-8-14-11-6-4-3-5-7-11/h3-7,10H,8-9H2,1-2H3
InchiKey:	MJTPMXWJHPOWGH-UHFFFAOYSA-N
Formula:	C12H16O3
SMILES:	CC(C)C(=O)OCCOc1ccccc1
Mol. weight [g/mol]:	208.25
CAS:	103-60-6

Physical Properties

Property code	Value	Unit	Source
gf	-178.79	kJ/mol	Joback Method
hf	-436.78	kJ/mol	Joback Method
hfus	21.33	kJ/mol	Joback Method
hvap	55.76	kJ/mol	Joback Method
log10ws	-2.31		Crippen Method
logp	2.265		Crippen Method
mcvol	169.490	ml/mol	McGowan Method
pc	2495.01	kPa	Joback Method
rinpol	1482.50		NIST Webbook
rinpol	1493.00		NIST Webbook
rinpol	1482.50		NIST Webbook
rinpol	1493.00		NIST Webbook
ripol	2100.00		NIST Webbook
ripol	2100.00		NIST Webbook
ripol	2106.00		NIST Webbook
tb	598.91	K	Joback Method
tc	806.97	K	Joback Method
tf	330.81	K	Joback Method
vc	0.635	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	420.15	J/mol×K	598.91	Joback Method
cpg	435.37	J/mol×K	633.59	Joback Method
cpg	449.74	J/mol×K	668.26	Joback Method
cpg	463.27	J/mol×K	702.94	Joback Method
cpg	475.99	J/mol×K	737.62	Joback Method
cpg	487.88	J/mol×K	772.30	Joback Method
cpg	498.98	J/mol×K	806.97	Joback Method
dvisc	0.0020694	Pa×s	330.81	Joback Method
dvisc	0.0010071	Pa×s	375.49	Joback Method
dvisc	0.0005713	Pa×s	420.18	Joback Method
dvisc	0.0003614	Pa×s	464.86	Joback Method
dvisc	0.0002477	Pa×s	509.54	Joback Method
dvisc	0.0001805	Pa×s	554.23	Joback Method
dvisc	0.0001378	Pa×s	598.91	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C103606&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume