3-Phenoxypropionic acid

Other names: 3-Phenoxypropanoic acid
«beta»-Phenoxypropionic acid
Propanoic acid, 3-phenoxy-
Inchi: InChI=1S/C9H10O3/c10-9(11)6-7-12-8-4-2-1-3-5-8/h1-5H,6-7H2,(H,10,11)
InchiKey: BUSOTUQRURCMCM-UHFFFAOYSA-N
Formula: C9H10O3
SMILES: O=C(O)CCOc1ccccc1
Mol. weight [g/mol]: 166.17
CAS: 7170-38-9

Physical Properties

Property code	Value	Unit	Source
gf	-233.43	kJ/mol	Joback Method
hf	-389.59	kJ/mol	Joback Method
hfus	19.98	kJ/mol	Joback Method
hvap	63.74	kJ/mol	Joback Method
log10ws	-1.53		Crippen Method
logp	1.540		Crippen Method
mcvol	127.220	ml/mol	McGowan Method
pc	3843.54	kPa	Joback Method
tb	513.20	K	NIST Webbook
tc	801.75	K	Joback Method
tf	350.59	K	Joback Method
vc	0.474	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	304.10	J/mol×K	600.47	Joback Method
cpg	349.97	J/mol×K	768.21	Joback Method
cpg	341.95	J/mol×K	734.66	Joback Method
cpg	333.37	J/mol×K	701.11	Joback Method
cpg	324.21	J/mol×K	667.56	Joback Method
cpg	314.46	J/mol×K	634.02	Joback Method

cpg	357.45	J/mol×K	801.75	Joback Method
dvisc	0.0000813	Pa×s	600.47	Joback Method
dvisc	0.0001222	Pa×s	558.82	Joback Method
dvisc	0.0001960	Pa×s	517.18	Joback Method
dvisc	0.0003415	Pa×s	475.53	Joback Method
dvisc	0.0006620	Pa×s	433.88	Joback Method
dvisc	0.0014770	Pa×s	392.24	Joback Method
dvisc	0.0039872	Pa×s	350.59	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C7170389&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
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume