Propanoic acid, 2-phenoxy-, (.+/-.)-

Inchi: InChI=1S/C9H10O3/c1-7(9(10)11)12-8-5-3-2-4-6-8/h2-7H,1H3,(H,10,11)
InchiKey: SXERGJJQSKIUIC-UHFFFAOYSA-N
Formula: C9H10O3
SMILES: CC(Oc1ccccc1)C(=O)O
Mol. weight [g/mol]: 166.17
CAS: 1912-21-6

Physical Properties

Property code	Value	Unit	Source
gf	-235.87	kJ/mol	Joback Method
hf	-394.87	kJ/mol	Joback Method
hfus	16.46	kJ/mol	Joback Method
hvap	63.35	kJ/mol	Joback Method
log10ws	-1.64		Crippen Method
logp	1.538		Crippen Method
mcvol	127.220	ml/mol	McGowan Method
pc	3881.95	kPa	Joback Method
tb	538.70	K	NIST Webbook
tc	805.31	K	Joback Method
tf	335.59	K	Joback Method
vc	0.469	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	304.57	J/mol×K	600.03	Joback Method
cpg	351.39	J/mol×K	771.10	Joback Method
cpg	343.24	J/mol×K	736.89	Joback Method
cpg	334.50	J/mol×K	702.67	Joback Method
cpg	325.16	J/mol×K	668.46	Joback Method
cpg	315.18	J/mol×K	634.24	Joback Method
cpg	358.96	J/mol×K	805.31	Joback Method
dvisc	0.0000761	Pa×s	600.03	Joback Method
dvisc	0.0001179	Pa×s	555.96	Joback Method

dvisc	0.0001971	Pa×s	511.88	Joback Method
dvisc	0.0003629	Pa×s	467.81	Joback Method
dvisc	0.0007586	Pa×s	423.74	Joback Method
dvisc	0.0018822	Pa×s	379.66	Joback Method
dvisc	0.0059290	Pa×s	335.59	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	378.70	K	0.70	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1912216&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
tb: Normal Boiling Point Temperature
tbrp: Boiling point at reduced pressure
tc: Critical Temperature
tf: Normal melting (fusion) point

vc: Critical Volume