4-Phenoxybenzaldehyde

Other names:	p-Phenoxybenzaldehyde
	Benzaldehyde, 4-phenoxy-
	Benzaldehyde, p-phenoxy-
Inchi:	InChI=1S/C13H10O2/c14-10-11-6-8-13(9-7-11)15-12-4-2-1-3-5-12/h1-10H
InchiKey:	QWLHJVDRPZNVBS-UHFFFAOYSA-N
Formula:	C13H10O2
SMILES:	O=Cc1ccc(Oc2ccccc2)cc1
Mol. weight [g/mol]:	198.22
CAS:	67-36-7

Physical Properties

Property code	Value	Unit	Source
gf	69.25	kJ/mol	Joback Method
hf	-67.86	kJ/mol	Joback Method
hfus	20.60	kJ/mol	Joback Method
hvap	58.88	kJ/mol	Joback Method
log10ws	-3.35		Crippen Method
logp	3.291		Crippen Method
mcvol	153.950	ml/mol	McGowan Method
pc	3220.98	kPa	Joback Method
rinpol	294.90		NIST Webbook
tb	626.26	K	Joback Method
tc	869.78	K	Joback Method
tf	365.86	K	Joback Method
vc	0.583	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	366.39	J/mol×K	626.26	Joback Method
cpg	426.63	J/mol×K	829.19	Joback Method
cpg	416.61	J/mol×K	788.61	Joback Method
cpg	405.62	J/mol×K	748.02	Joback Method
cpg	393.62	J/mol×K	707.43	Joback Method

cpg	380.55	J/mol×K	666.85	Joback Method
cpg	435.72	J/mol×K	869.78	Joback Method
dvisc	0.0001812	Pa×s	626.26	Joback Method
dvisc	0.0002262	Pa×s	582.86	Joback Method
dvisc	0.0002926	Pa×s	539.46	Joback Method
dvisc	0.0003959	Pa×s	496.06	Joback Method
dvisc	0.0005677	Pa×s	452.66	Joback Method
dvisc	0.0008787	Pa×s	409.26	Joback Method
dvisc	0.0015087	Pa×s	365.86	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	458.20	K	1.90	NIST Webbook

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C67367&Units=SI

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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume