p-Phenoxystyrene

Other names: p-Phenoxystyrene
4-Phenoxystyrene
Inchi: InChI=1S/C14H12O/c1-2-12-8-10-14(11-9-12)15-13-6-4-3-5-7-13/h2-11H,1H2
InchiKey: UULPGUKSBAXNJN-UHFFFAOYSA-N
Formula: C14H12O
SMILES: C=Cc1ccc(Oc2ccccc2)cc1
Mol. weight [g/mol]: 196.25

Physical Properties

Property code	Value	Unit	Source
af	0.5015		Cheméo Relay (1.0)
hf	121.84	kJ/mol	Cheméo Relay (1.0)
hfus	19.62	kJ/mol	Joback Method
hvap	74.40	kJ/mol	Cheméo Relay (1.0)
ie	7.61	eV	Cheméo Relay (1.0)
log10ws	-4.51		Cheméo Relay (1.0)
logp	4.122		Crippen Method
mcvol	162.170	ml/mol	McGowan Method
pc	2799.47	kPa	Joback Method
tb	574.07	K	Cheméo Relay (1.0)
tc	821.12	K	Cheméo Relay (1.0)
tf	315.26	K	Cheméo Relay (1.0)
vc	0.587	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	376.86	J/mol×K	597.16	Joback Method
cpg	393.09	J/mol×K	637.55	Joback Method
cpg	408.11	J/mol×K	677.95	Joback Method
cpg	421.98	J/mol×K	718.34	Joback Method
cpg	434.75	J/mol×K	758.73	Joback Method
cpg	446.50	J/mol×K	799.13	Joback Method
cpg	457.26	J/mol×K	839.52	Joback Method

dvisc	0.0014038	Pa×s	333.37	Joback Method
dvisc	0.0007746	Pa×s	377.34	Joback Method
dvisc	0.0004839	Pa×s	421.30	Joback Method
dvisc	0.0003304	Pa×s	465.27	Joback Method
dvisc	0.0002410	Pa×s	509.23	Joback Method
dvisc	0.0001848	Pa×s	553.20	Joback Method
dvisc	0.0001473	Pa×s	597.16	Joback Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C4973299&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Legend

af: Acentric Factor
cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hvap: Enthalpy of vaporization at standard conditions
ie: Ionization energy
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