S-(-)-1-phenylpropanol

Inchi: InChI=1S/C9H12O/c1-2-9(10)8-6-4-3-5-7-8/h3-7,9-10H,2H2,1H3/t9-/m0/s1
InchiKey: DYUQAZSOFZSPHD-SECBINFHSA-N
Formula: C9H12O
SMILES: CC[C@H](O)c1ccccc1
Mol. weight [g/mol]: 136.19

Physical Properties

Property code	Value	Unit	Source
af	0.5477		Cheméo Relay (1.0)
gf	-1.95	kJ/mol	Joback Method
hf	-169.12	kJ/mol	Cheméo Relay (1.0)
hfus	13.67	kJ/mol	Joback Method
hvap	68.83	kJ/mol	Cheméo Relay (1.0)
ie	9.13	eV	Cheméo Relay (1.0)
log10ws	-1.41		Cheméo Relay (1.0)
logp	2.130		Crippen Method
mcvol	119.780	ml/mol	McGowan Method
pc	3668.65	kPa	Joback Method
tb	478.97	K	Cheméo Relay (1.0)
tc	696.72	K	Cheméo Relay (1.0)
tf	316.60	K	Cheméo Relay (1.0)
vc	0.439	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	267.01	J/mol×K	523.74	Joback Method
cpg	278.99	J/mol×K	556.92	Joback Method
cpg	290.28	J/mol×K	590.10	Joback Method
cpg	300.91	J/mol×K	623.28	Joback Method
cpg	310.91	J/mol×K	656.46	Joback Method
cpg	320.31	J/mol×K	689.65	Joback Method
cpg	329.13	J/mol×K	722.83	Joback Method
dvisc	0.0307952	Pa×s	263.43	Joback Method

dvisc	0.0063252	Pa×s	306.81	Joback Method
dvisc	0.0019230	Pa×s	350.20	Joback Method
dvisc	0.0007602	Pa×s	393.59	Joback Method
dvisc	0.0003613	Pa×s	436.97	Joback Method
dvisc	0.0001964	Pa×s	480.36	Joback Method
dvisc	0.0001181	Pa×s	523.74	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C613876&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):
Cheméo Relay (1.0, beta):

Legend

af: Acentric Factor
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
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