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-/m1/s1
InchiKey: DYUQAZSOFZSPHD-SECBINFHSA-N
Formula: C9H12O
SMILES: CCC(O)c1ccccc1
Mol. weight [g/mol]: 136.19
CAS: 613-87-6

Physical Properties

Property code	Value	Unit	Source
gf	-1.95	kJ/mol	Joback Method
hf	-150.07	kJ/mol	Joback Method
hfus	13.67	kJ/mol	Joback Method
hvap	54.19	kJ/mol	Joback Method
log10ws	-2.42		Crippen Method
logp	2.130		Crippen Method
mcvol	119.780	ml/mol	McGowan Method
pc	3668.65	kPa	Joback Method
tb	523.74	K	Joback Method
tc	722.83	K	Joback Method
tf	263.43	K	Joback Method
vc	0.445	m3/kmol	Joback Method

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

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=C613876&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume