

Phenylpropanol

Inchi:	InChI=1S/C9H12O/c10-8-4-7-9-5-2-1-3-6-9/h1-3,5-6,10H,4,7-8H2
InchiKey:	VAJVDSVGBWFCLW-UHFFFAOYSA-N
Formula:	C9H12O
SMILES:	OCCCC1CCCCC1
Mol. weight [g/mol]:	136.19
CAS:	93842-54-7

Physical Properties

Property code	Value	Unit	Source
gf	0.49	kJ/mol	Joback Method
hf	-144.79	kJ/mol	Joback Method
hfus	17.20	kJ/mol	Joback Method
hvap	54.58	kJ/mol	Joback Method
log10ws	-1.96		Crippen Method
logp	1.611		Crippen Method
mcvol	119.780	ml/mol	McGowan Method
pc	3633.35	kPa	Joback Method
ripol	1980.00		NIST Webbook
tb	524.18	K	Joback Method
tc	719.09	K	Joback Method
tf	278.43	K	Joback Method
vc	0.451	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	266.71	J/mol×K	524.18	Joback Method
cpg	278.37	J/mol×K	556.66	Joback Method
cpg	289.37	J/mol×K	589.15	Joback Method
cpg	299.75	J/mol×K	621.63	Joback Method
cpg	309.54	J/mol×K	654.12	Joback Method
cpg	318.76	J/mol×K	686.60	Joback Method
cpg	327.43	J/mol×K	719.09	Joback Method
dvisc	0.0168187	Pa×s	278.43	Joback Method

dvisc	0.0044008	Pa×s	319.39	Joback Method
dvisc	0.0015618	Pa×s	360.35	Joback Method
dvisc	0.0006848	Pa×s	401.30	Joback Method
dvisc	0.0003498	Pa×s	442.26	Joback Method
dvisc	0.0002002	Pa×s	483.22	Joback Method
dvisc	0.0001251	Pa×s	524.18	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C93842547&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

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:

<https://www.chemeo.com/cid/71-324-3/Phenylpropanol.pdf>

Generated by Cheméo on 2025-12-23 16:22:52.785530897 +0000 UTC m=+6255170.315571551.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.