C9H12O

Inchi: InChI=1S/C9H12O/c1-7-4-3-5-9(6-7)8(2)10/h3-6,8,10H,1-2H3
InchiKey: SPNHUMWMKXWVIU-UHFFFAOYSA-N
Formula: C9H12O
SMILES: Cc1cccc(C(C)O)c1
Mol. weight [g/mol]: 136.19
CAS: 25675-28-9

Physical Properties

Property code	Value	Unit	Source
gf	-11.58	kJ/mol	Joback Method
hf	-161.54	kJ/mol	Joback Method
hfus	13.28	kJ/mol	Joback Method
hvap	54.86	kJ/mol	Joback Method
log10ws	-2.47		Crippen Method
logp	2.048		Crippen Method
mcvol	119.780	ml/mol	McGowan Method
pc	3602.88	kPa	Joback Method
tb	528.72	K	Joback Method
tc	728.91	K	Joback Method
tf	275.95	K	Joback Method
vc	0.445	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	266.77	J/mol×K	528.72	Joback Method
cpg	278.42	J/mol×K	562.08	Joback Method
cpg	289.43	J/mol×K	595.45	Joback Method
cpg	299.83	J/mol×K	628.81	Joback Method
cpg	309.65	J/mol×K	662.18	Joback Method
cpg	318.90	J/mol×K	695.54	Joback Method
cpg	327.61	J/mol×K	728.91	Joback Method
dvisc	0.0169073	Pa×s	275.95	Joback Method
dvisc	0.0042083	Pa×s	318.08	Joback Method

dvisc	0.0014502	Pa×s	360.21	Joback Method
dvisc	0.0006246	Pa×s	402.34	Joback Method
dvisc	0.0003156	Pa×s	444.46	Joback Method
dvisc	0.0001795	Pa×s	486.59	Joback Method
dvisc	0.0001117	Pa×s	528.72	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C25675289&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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