1,2,3,6-Tetrahydrobenzylalcohol, acetate

Other names: Cyclohexen-4-methanol, acetate
Inchi: InChI=1S/C9H14O2/c1-8(10)11-7-9-5-3-2-4-6-9/h2-3,9H,4-7H2,1H3
InchiKey: UYBXBOOBIVAIJM-UHFFFAOYSA-N
Formula: C9H14O2
SMILES: CC(=O)OCC1CC=CCC1
Mol. weight [g/mol]: 154.21

Physical Properties

Property code	Value	Unit	Source
gf	-154.61	kJ/mol	Joback Method
hf	-361.79	kJ/mol	Joback Method
hfus	14.91	kJ/mol	Joback Method
hvap	45.51	kJ/mol	Joback Method
log10ws	-1.96		Crippen Method
logp	1.906		Crippen Method
mcvol	129.950	ml/mol	McGowan Method
pc	3103.64	kPa	Joback Method
rinpol	1141.00		NIST Webbook
rinpol	1141.00		NIST Webbook
tb	500.32	K	Joback Method
tc	710.84	K	Joback Method
tf	271.49	K	Joback Method
vc	0.482	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	291.39	J/mol×K	500.32	Joback Method
cpg	307.24	J/mol×K	535.41	Joback Method
cpg	322.28	J/mol×K	570.49	Joback Method
cpg	336.51	J/mol×K	605.58	Joback Method
cpg	349.96	J/mol×K	640.67	Joback Method
cpg	362.62	J/mol×K	675.75	Joback Method
cpg	374.52	J/mol×K	710.84	Joback Method

dvisc	0.0035591	Pa×s	271.49	Joback Method
dvisc	0.0017580	Pa×s	309.63	Joback Method
dvisc	0.0010136	Pa×s	347.77	Joback Method
dvisc	0.0006516	Pa×s	385.90	Joback Method
dvisc	0.0004536	Pa×s	424.04	Joback Method
dvisc	0.0003352	Pa×s	462.18	Joback Method
dvisc	0.0002593	Pa×s	500.32	Joback Method

Sources

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=U365586&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume