5-Hexene-1-ol, acetate

Other names:	Acetic acid 5-hexenyl ester
	5-Hexen-1-ol, acetate
	5-hexenyl acetate
	5-Hexen-1-ol, 1-acetate
Inchi:	InChI=1S/C8H14O2/c1-3-4-5-6-7-10-8(2)9/h3H,1,4-7H2,2H3
InchiKey:	MPLWNENKBSBMFN-UHFFFAOYSA-N
Formula:	C8H14O2
SMILES:	C=CCCCCOC(C)=O
Mol. weight [g/mol]:	142.20
CAS:	5048-26-0

Physical Properties

Property code	Value	Unit	Source
gf	-129.60	kJ/mol	Joback Method
hf	-327.82	kJ/mol	Joback Method
hfus	17.98	kJ/mol	Joback Method
hvap	41.89	kJ/mol	Joback Method
log10ws	-1.89		Crippen Method
logp	1.906		Crippen Method
mcvol	126.720	ml/mol	McGowan Method
pc	2775.92	kPa	Joback Method
rinpol	1001.40		NIST Webbook
ripol	1313.00		NIST Webbook
ripol	1313.00		NIST Webbook
ripol	1313.00		NIST Webbook
ripol	1313.00		NIST Webbook
tb	455.41	K	Joback Method
tc	633.98	K	Joback Method
tf	250.32	K	Joback Method
vc	0.488	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	263.07	J/mol×K	455.41	Joback Method
cpg	316.89	J/mol×K	604.22	Joback Method
cpg	306.99	J/mol×K	574.46	Joback Method
cpg	296.66	J/mol×K	544.69	Joback Method
cpg	285.90	J/mol×K	514.93	Joback Method
cpg	274.71	J/mol×K	485.17	Joback Method
cpg	326.37	J/mol×K	633.98	Joback Method
dvisc	0.0002547	Pa×s	455.41	Joback Method
dvisc	0.0003249	Pa×s	421.23	Joback Method
dvisc	0.0004328	Pa×s	387.05	Joback Method
dvisc	0.0006093	Pa×s	352.87	Joback Method
dvisc	0.0009231	Pa×s	318.68	Joback Method
dvisc	0.0015454	Pa×s	284.50	Joback Method
dvisc	0.0029783	Pa×s	250.32	Joback Method

Sources

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=C5048260&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature

tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume