3,7-Dimethyl-6-nonen-1-ol acetate

Inchi: InChI=1S/C13H24O2/c1-5-11(2)7-6-8-12(3)9-10-15-13(4)14/h7,12H,5-6,8-10H2,1-4H3/b
InchiKey: XWIYCKNKJXJOIR-YRNVUSSQSA-N
Formula: C13H24O2
SMILES: CCC(C)=CCCC(C)CCOC(C)=O
Mol. weight [g/mol]: 212.33

Physical Properties

Property code	Value	Unit	Source
gf	-106.11	kJ/mol	Joback Method
hf	-454.30	kJ/mol	Joback Method
hfus	27.58	kJ/mol	Joback Method
hvap	53.34	kJ/mol	Joback Method
log10ws	-3.74		Crippen Method
logp	3.712		Crippen Method
mcvol	197.170	ml/mol	McGowan Method
pc	1803.09	kPa	Joback Method
rinpol	1614.00		NIST Webbook
tb	576.73	K	Joback Method
tc	757.65	K	Joback Method
tf	274.39	K	Joback Method
vc	0.762	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	495.91	J/mol×K	576.73	Joback Method
cpg	512.41	J/mol×K	606.88	Joback Method
cpg	528.17	J/mol×K	637.04	Joback Method
cpg	543.21	J/mol×K	667.19	Joback Method
cpg	557.54	J/mol×K	697.35	Joback Method
cpg	571.19	J/mol×K	727.50	Joback Method
cpg	584.19	J/mol×K	757.65	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U131349&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
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