(Z,Z)-3,6-nonadienyl acetate

Inchi: InChI=1S/C11H18O2/c1-3-4-5-6-7-8-9-10-13-11(2)12/h4-5,7-8H,3,6,9-10H2,1-2H3/b5-4-
InchiKey: CMNKZQXSZSHGNF-UTOQUPLUSA-N
Formula: C11H18O2
SMILES: CCC=CCC=CCCOC(C)=O
Mol. weight [g/mol]: 182.26

Physical Properties

Property code	Value	Unit	Source
gf	-31.74	kJ/mol	Joback Method
hf	-280.73	kJ/mol	Joback Method
hfus	27.44	kJ/mol	Joback Method
hvap	49.15	kJ/mol	Joback Method
log10ws	-3.00		Crippen Method
logp	2.852		Crippen Method
mcvol	164.690	ml/mol	McGowan Method
pc	2216.62	kPa	Joback Method
tb	535.69	K	Joback Method
tc	721.31	K	Joback Method
tf	275.73	K	Joback Method
vc	0.635	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	379.20	J/mol×K	535.69	Joback Method
cpg	393.43	J/mol×K	566.63	Joback Method
cpg	406.97	J/mol×K	597.56	Joback Method
cpg	419.86	J/mol×K	628.50	Joback Method
cpg	432.12	J/mol×K	659.44	Joback Method
cpg	443.78	J/mol×K	690.38	Joback Method
cpg	454.86	J/mol×K	721.31	Joback Method
dvisc	0.0027700	Pa×s	275.73	Joback Method
dvisc	0.0012188	Pa×s	319.06	Joback Method
dvisc	0.0006526	Pa×s	362.38	Joback Method

dvisc	0.0003993	Pa×s	405.71	Joback Method
dvisc	0.0002686	Pa×s	449.04	Joback Method
dvisc	0.0001938	Pa×s	492.36	Joback Method
dvisc	0.0001473	Pa×s	535.69	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R308053&Units=SI

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

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