

3-6-Nonadien-1-yl-acetate

Other names:	3,6-Nonadien-1-ol, acetate 3,6-Nonadienyl acetate nona-3,6-dienyl 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-AOSYACOCSA-N
Formula:	C11H18O2
SMILES:	CCC=CCC=CCOC(C)=O
Mol. weight [g/mol]:	182.26
CAS:	76649-26-8

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
ripol	1676.00		NIST Webbook
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/molxK	535.69	Joback Method
cpg	393.43	J/molxK	566.63	Joback Method
cpg	406.97	J/molxK	597.56	Joback Method
cpg	419.86	J/molxK	628.50	Joback Method
cpg	432.12	J/molxK	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	Paxs	275.73	Joback Method
dvisc	0.0012188	Paxs	319.06	Joback Method
dvisc	0.0006526	Paxs	362.38	Joback Method
dvisc	0.0003993	Paxs	405.71	Joback Method
dvisc	0.0002686	Paxs	449.04	Joback Method
dvisc	0.0001938	Paxs	492.36	Joback Method
dvisc	0.0001473	Paxs	535.69	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C76649268&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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