

2-Nonadecanone-1-ol, acetate

Inchi: InChI=1S/C21H40O3/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-21(23)19-24-20(2)22
InchiKey: SWPXNKMHYMFQCW-UHFFFAOYSA-N
Formula: C21H40O3
SMILES: CCCCCCCCCCCCCCCCCC(=O)COC(C)=O
Mol. weight [g/mol]: 340.54

Physical Properties

Property code	Value	Unit	Source
gf	-236.90	kJ/mol	Joback Method
hf	-834.15	kJ/mol	Joback Method
hfus	54.53	kJ/mol	Joback Method
hvap	78.24	kJ/mol	Joback Method
log10ws	-6.76		Crippen Method
logp	6.380		Crippen Method
mcvol	315.760	ml/mol	McGowan Method
pc	1024.00	kPa	Joback Method
tb	810.04	K	Joback Method
tc	993.68	K	Joback Method
tf	448.52	K	Joback Method
vc	1.242	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	998.13	J/molxK	810.04	Joback Method
cpg	1017.01	J/molxK	840.65	Joback Method
cpg	1034.86	J/molxK	871.25	Joback Method
cpg	1051.71	J/molxK	901.86	Joback Method
cpg	1067.58	J/molxK	932.47	Joback Method
cpg	1082.50	J/molxK	963.08	Joback Method
cpg	1096.50	J/molxK	993.68	Joback Method
dvisc	0.0011053	Paxs	448.52	Joback Method
dvisc	0.0005136	Paxs	508.77	Joback Method
dvisc	0.0002808	Paxs	569.03	Joback Method

dvisc	0.0001723	Paxs	629.28	Joback Method
dvisc	0.0001151	Paxs	689.53	Joback Method
dvisc	0.0000821	Paxs	749.79	Joback Method
dvisc	0.0000616	Paxs	810.04	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=B6002029&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
hvac:	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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