

Acetoxyacetic acid, nonyl ester

Inchi:	InChI=1S/C13H24O4/c1-3-4-5-6-7-8-9-10-16-13(15)11-17-12(2)14/h3-11H2,1-2H3
InchiKey:	XTGNORUZGLCPJZ-UHFFFAOYSA-N
Formula:	C13H24O4
SMILES:	CCCCCCCCCOC(=O)COC(C)=O
Mol. weight [g/mol]:	244.33

Physical Properties

Property code	Value	Unit	Source
gf	-409.26	kJ/mol	Joback Method
hf	-801.25	kJ/mol	Joback Method
hfus	35.00	kJ/mol	Joback Method
hvap	62.84	kJ/mol	Joback Method
log10ws	-2.99		Crippen Method
logp	2.843		Crippen Method
mcvol	208.910	ml/mol	McGowan Method
pc	1774.35	kPa	Joback Method
rinsol	1631.00		NIST Webbook
tb	649.42	K	Joback Method
tc	825.90	K	Joback Method
tf	380.59	K	Joback Method
vc	0.811	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	568.37	J/molxK	649.42	Joback Method
cpg	583.50	J/molxK	678.83	Joback Method
cpg	597.94	J/molxK	708.25	Joback Method
cpg	611.72	J/molxK	737.66	Joback Method
cpg	624.81	J/molxK	767.07	Joback Method
cpg	637.24	J/molxK	796.48	Joback Method
cpg	649.00	J/molxK	825.90	Joback Method
dvisc	0.0016009	Paxs	380.59	Joback Method
dvisc	0.0008539	Paxs	425.40	Joback Method

dvisc	0.0005134	Paxs	470.20	Joback Method
dvisc	0.0003373	Paxs	515.00	Joback Method
dvisc	0.0002370	Paxs	559.81	Joback Method
dvisc	0.0001754	Paxs	604.62	Joback Method
dvisc	0.0001354	Paxs	649.42	Joback Method

Sources

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=U308314&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

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