

10-Acetoxyneryl acetate

Inchi:	InChI=1S/C14H22O4/c1-11(2)6-5-7-14(10-18-13(4)16)8-9-17-12(3)15/h6,8H,5,7,9-10H2,
InchiKey:	BGMGTQUWFVQNBG-RIYZIHGNSA-N
Formula:	C14H22O4
SMILES:	CC(=O)OCC=C(CCC=C(C)C)COC(C)=O
Mol. weight [g/mol]:	254.32

Physical Properties

Property code	Value	Unit	Source
gf	-257.50	kJ/mol	Joback Method
hf	-607.03	kJ/mol	Joback Method
hfus	35.37	kJ/mol	Joback Method
hvap	65.15	kJ/mol	Joback Method
log10ws	-3.12		Crippen Method
logp	2.785		Crippen Method
mvol	214.400	ml/mol	McGowan Method
pc	1801.56	kPa	Joback Method
ripol	1660.00		NIST Webbook
ripol	2325.00		NIST Webbook
tb	680.38	K	Joback Method
tc	872.22	K	Joback Method
tf	353.78	K	Joback Method
vc	0.830	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	577.21	J/mol×K	680.38	Joback Method
cpg	592.19	J/mol×K	712.35	Joback Method
cpg	606.40	J/mol×K	744.33	Joback Method
cpg	619.85	J/mol×K	776.30	Joback Method
cpg	632.57	J/mol×K	808.27	Joback Method
cpg	644.59	J/mol×K	840.24	Joback Method
cpg	655.92	J/mol×K	872.22	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=R518166&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

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
rinpolar:	Non-polar retention indices
ripolar:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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