

Elemol acetate

Other names:	elemyl acetate «alpha»-Acetoxyelemol
Inchi:	InChI=1S/C17H28O2/c1-8-17(7)10-9-14(11-15(17)12(2)3)16(5,6)19-13(4)18/h8,14-15H,1
InchiKey:	WIOCBQJVVCZHFB-VYDXJSESSA-N
Formula:	C17H28O2
SMILES:	<chem>C=CC1(C)CCC(C(C)(C)OC(C)=O)CC1C(=C)C</chem>
Mol. weight [g/mol]:	264.40
CAS:	60031-93-8

Physical Properties

Property code	Value	Unit	Source
gf	31.85	kJ/mol	Joback Method
hf	-377.81	kJ/mol	Joback Method
hfus	18.97	kJ/mol	Joback Method
hvap	58.70	kJ/mol	Joback Method
log10ws	-4.79		Crippen Method
logp	4.513		Crippen Method
mcvol	238.370	ml/mol	McGowan Method
pc	1584.75	kPa	Joback Method
rinpol	1675.10		NIST Webbook
rinpol	1679.00		NIST Webbook
rinpol	1691.00		NIST Webbook
rinpol	1679.00		NIST Webbook
rinpol	1675.10		NIST Webbook
ripol	2026.00		NIST Webbook
tb	665.11	K	Joback Method
tc	878.70	K	Joback Method
tf	361.25	K	Joback Method
vc	0.892	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	682.00	J/mol×K	665.11	Joback Method

cpg	703.90	J/mol×K	700.71	Joback Method
cpg	724.61	J/mol×K	736.31	Joback Method
cpg	744.26	J/mol×K	771.90	Joback Method
cpg	762.99	J/mol×K	807.50	Joback Method
cpg	780.91	J/mol×K	843.10	Joback Method
cpg	798.18	J/mol×K	878.70	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C60031938&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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

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