

Z-(13,14-Epoxy)tetradec-11-en-1-ol acetate

Other names:	(Z)-11-(13,14-Epoxy)tetradecen-1-ol acetate
Inchi:	InChI=1S/C16H28O3/c1-15(17)18-13-11-9-7-5-3-2-4-6-8-10-12-16-14-19-16/h10,12,16H
InchiKey:	SSNSHVODQWMOJI-BENRWUELSA-N
Formula:	C16H28O3
SMILES:	CC(=O)OCCCCCCCCCCC=CC1CO1
Mol. weight [g/mol]:	268.39

Physical Properties

Property code	Value	Unit	Source
gf	-95.23	kJ/mol	Joback Method
hf	-560.35	kJ/mol	Joback Method
hfus	46.30	kJ/mol	Joback Method
hvap	64.75	kJ/mol	Joback Method
log10ws	-4.33		Crippen Method
logp	4.015		Crippen Method
mvol	234.450	ml/mol	McGowan Method
pc	1556.12	kPa	Joback Method
rinpol	1849.00		NIST Webbook
rinpol	1849.00		NIST Webbook
tb	679.62	K	Joback Method
tc	861.39	K	Joback Method
tf	381.67	K	Joback Method
vc	0.913	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	676.26	J/mol×K	679.62	Joback Method
cpg	693.47	J/mol×K	709.91	Joback Method
cpg	709.83	J/mol×K	740.21	Joback Method
cpg	725.37	J/mol×K	770.50	Joback Method
cpg	740.14	J/mol×K	800.80	Joback Method
cpg	754.17	J/mol×K	831.09	Joback Method
cpg	767.52	J/mol×K	861.39	Joback Method

dvisc	0.0021715	Paxs	381.67	Joback Method
dvisc	0.0012344	Paxs	431.33	Joback Method
dvisc	0.0007885	Paxs	480.99	Joback Method
dvisc	0.0005477	Paxs	530.64	Joback Method
dvisc	0.0004050	Paxs	580.30	Joback Method
dvisc	0.0003140	Paxs	629.96	Joback Method
dvisc	0.0002527	Paxs	679.62	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=U131332&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

Legend

cp_g:	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
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
log_p:	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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