

Artemisia acetate

Other names:	Artemisyl acetate Artemisia alcohol acetate 2,5,5-trimethylhepta-2,6-dien-4-yl acetate
Inchi:	InChI=1S/C12H20O2/c1-7-12(5,6)11(8-9(2)3)14-10(4)13/h7-8,11H,1H2,2-6H3
InchiKey:	NGIKFWJEQGLTBM-UHFFFAOYSA-N
Formula:	C12H20O2
SMILES:	<chem>C=CC(C)(C)C(C=C(C)C)OC(C)=O</chem>
Mol. weight [g/mol]:	196.29
CAS:	3465-88-1

Physical Properties

Property code	Value	Unit	Source
gf	-23.85	kJ/mol	Joback Method
hf	-316.98	kJ/mol	Joback Method
hfus	16.30	kJ/mol	Joback Method
hvap	49.15	kJ/mol	Joback Method
log10ws	-3.29		Crippen Method
logp	3.096		Crippen Method
mcvol	178.780	ml/mol	McGowan Method
pc	2069.88	kPa	Joback Method
rinpol	1158.00		NIST Webbook
rinpol	1190.00		NIST Webbook
rinpol	1172.00		NIST Webbook
rinpol	1152.00		NIST Webbook
rinpol	1172.00		NIST Webbook
rinpol	1173.00		NIST Webbook
rinpol	1161.00		NIST Webbook
rinpol	1174.10		NIST Webbook
rinpol	1172.00		NIST Webbook
rinpol	1155.00		NIST Webbook
rinpol	1164.00		NIST Webbook
rinpol	1172.00		NIST Webbook
rinpol	1173.00		NIST Webbook
rinpol	1173.00		NIST Webbook
rinpol	1153.00		NIST Webbook
ripol	1390.00		NIST Webbook
ripol	1417.00		NIST Webbook

ripol	1390.00		NIST Webbook
ripol	1404.00		NIST Webbook
ripol	1433.00		NIST Webbook
tb	547.30	K	Joback Method
tc	744.21	K	Joback Method
tf	263.78	K	Joback Method
vc	0.676	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	429.09	J/mol×K	547.30	Joback Method
cpg	445.42	J/mol×K	580.12	Joback Method
cpg	460.82	J/mol×K	612.94	Joback Method
cpg	475.36	J/mol×K	645.76	Joback Method
cpg	489.07	J/mol×K	678.57	Joback Method
cpg	501.99	J/mol×K	711.39	Joback Method
cpg	514.17	J/mol×K	744.21	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=C3465881&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
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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