

Artemiseole

Other names:	1,6,6-Trimethyl-4-ethenyl-exo-2-oxabicyclo[3.1.0] hexane Artemiseol Artemiseole (Arthole)
Inchi:	InChI=1S/C10H16O/c1-5-7-8-9(2,3)11-6-10(7,8)4/h5,7-8H,1,6H2,2-4H3
InchiKey:	HHDOWVHECSBICN-UHFFFAOYSA-N
Formula:	C10H16O
SMILES:	C=CC1C2C(C)(C)OCC12C
Mol. weight [g/mol]:	152.23
CAS:	60485-46-3

Physical Properties

Property code	Value	Unit	Source
gf	130.14	kJ/mol	Joback Method
hf	-120.90	kJ/mol	Joback Method
hfus	14.17	kJ/mol	Joback Method
hvap	38.60	kJ/mol	Joback Method
log10ws	-2.13		Crippen Method
logp	2.234		Crippen Method
mcvol	131.610	ml/mol	McGowan Method
pc	2887.40	kPa	Joback Method
rinpol	967.00		NIST Webbook
rinpol	967.80		NIST Webbook
rinpol	967.00		NIST Webbook
tb	456.45	K	Joback Method
tc	666.60	K	Joback Method
tf	302.47	K	Joback Method
vc	0.505	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	304.89	J/mol×K	456.45	Joback Method
cpg	322.96	J/mol×K	491.47	Joback Method
cpg	339.40	J/mol×K	526.50	Joback Method

cpg	354.44	J/mol×K	561.52	Joback Method
cpg	368.28	J/mol×K	596.55	Joback Method
cpg	381.16	J/mol×K	631.57	Joback Method
cpg	393.29	J/mol×K	666.60	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C60485463&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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

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