

1,5-Heptadien-4-one, 3,3,6-trimethyl-

Other names:	Artemisia ketone Isoartemisia ketone 2,5,5-Trimethyl-2,6-heptadien-4-one Artemesia Artemesia ketone Hepta-1,5-dien-4-one, 3,3,6-trimethyl 3,3,6-trimethylhepta-1,5-dien-4-one
Inchi:	InChI=1S/C10H16O/c1-6-10(4,5)9(11)7-8(2)3/h6-7H,1H2,2-5H3
InchiKey:	OTYVBQZXUNBRTK-UHFFFAOYSA-N
Formula:	C10H16O
SMILES:	<chem>C=CC(C)(C)C(=O)C=C(C)C</chem>
Mol. weight [g/mol]:	152.23
CAS:	546-49-6

Physical Properties

Property code	Value	Unit	Source
gf	66.75	kJ/mol	Joback Method
hf	-138.20	kJ/mol	Joback Method
hfus	13.45	kJ/mol	Joback Method
hvap	42.67	kJ/mol	Joback Method
log10ws	-2.75		Crippen Method
logp	2.734		Crippen Method
mcvol	144.730	ml/mol	McGowan Method
pc	2507.52	kPa	Joback Method
rinpol	1069.00		NIST Webbook
rinpol	1070.00		NIST Webbook
rinpol	1040.00		NIST Webbook
rinpol	1061.00		NIST Webbook
rinpol	1064.00		NIST Webbook
rinpol	1062.00		NIST Webbook
rinpol	1044.00		NIST Webbook
rinpol	1046.00		NIST Webbook
rinpol	1062.00		NIST Webbook
rinpol	1044.00		NIST Webbook
rinpol	1088.00		NIST Webbook
rinpol	1040.00		NIST Webbook
rinpol	1060.00		NIST Webbook

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ripol	1335.00		NIST Webbook
ripol	1348.00		NIST Webbook
ripol	1328.00		NIST Webbook
ripol	1320.00		NIST Webbook
ripol	1345.00		NIST Webbook
tb	479.56	K	Joback Method
tc	679.09	K	Joback Method
tf	234.01	K	Joback Method
vc	0.552	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	310.37	J/mol×K	479.56	Joback Method
cpg	325.35	J/mol×K	512.81	Joback Method
cpg	339.41	J/mol×K	546.07	Joback Method
cpg	352.60	J/mol×K	579.32	Joback Method
cpg	364.97	J/mol×K	612.58	Joback Method
cpg	376.58	J/mol×K	645.83	Joback Method
cpg	387.47	J/mol×K	679.09	Joback Method

Sources

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C546496&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

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

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