

Myrcenyl acetate

Inchi:	InChI=1S/C12H20O2/c1-6-10(2)8-7-9-12(4,5)14-11(3)13/h6H,1-2,7-9H2,3-5H3
InchiKey:	DCXXKSXLKWAZNO-UHFFFAOYSA-N
Formula:	C12H20O2
SMILES:	C=CC(=C)CCCC(C)(C)OC(C)=O
Mol. weight [g/mol]:	196.29
CAS:	1118-39-4

Physical Properties

Property code	Value	Unit	Source
gf	-13.79	kJ/mol	Joback Method
hf	-303.49	kJ/mol	Joback Method
hfus	18.34	kJ/mol	Joback Method
hvap	48.91	kJ/mol	Joback Method
log10ws	-3.53		Crippen Method
logp	3.241		Crippen Method
mcvol	178.780	ml/mol	McGowan Method
pc	2036.39	kPa	Joback Method
rinpol	1246.00		NIST Webbook
rinpol	1247.00		NIST Webbook
rinpol	1261.00		NIST Webbook
ripol	1595.00		NIST Webbook
ripol	1574.00		NIST Webbook
ripol	1571.00		NIST Webbook
tb	540.26	K	Joback Method
tc	728.81	K	Joback Method
tf	282.10	K	Joback Method
vc	0.683	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	427.58	J/mol×K	540.26	Joback Method
cpg	443.36	J/mol×K	571.68	Joback Method
cpg	458.31	J/mol×K	603.11	Joback Method

cpg	472.48	J/mol×K	634.53	Joback Method
cpg	485.89	J/mol×K	665.96	Joback Method
cpg	498.57	J/mol×K	697.38	Joback Method
cpg	510.56	J/mol×K	728.81	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1118394&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
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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