

menthadien-2-yl acetate, p-1(7),8

Other names:	menthadien-2-yl acetate, p-1(7),8
Inchi:	InChI=1S/C12H18O2/c1-8(2)11-6-5-9(3)12(7-11)14-10(4)13/h11-12H,1,3,5-7H2,2,4H3
InchiKey:	CCLNPVCMIJDLR-UHFFFAOYSA-N
Formula:	C12H18O2
SMILES:	<chem>C=C(C)C1CCC(=C)C(OC(C)=O)C1</chem>
Mol. weight [g/mol]:	194.27

Physical Properties

Property code	Value	Unit	Source
hfus	18.78	kJ/mol	Joback Method
logp	2.850		Crippen Method
mcvol	167.920	ml/mol	McGowan Method
ripol	1763.00		NIST Webbook
tb	501.46	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	414.55	J/mol×K	560.85	Joback Method
cpg	432.66	J/mol×K	595.62	Joback Method
cpg	449.82	J/mol×K	630.38	Joback Method
cpg	466.06	J/mol×K	665.15	Joback Method
cpg	481.39	J/mol×K	699.92	Joback Method
cpg	495.80	J/mol×K	734.69	Joback Method
cpg	509.32	J/mol×K	769.45	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C1134969&Units=SI>

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
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
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature

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