

limonen-10-yl acetate

Other names:	p-mentha-1,8-dien-9-yl acetate 10-Limonenyl acetate p-mentha-1,8-dien-10-yl acetate 10-Limonenol, acetate limonene-10-yl acetate 4-methyl-«beta»-methylenecyclohex-3-ene-1-ethyl acetate
Inchi:	InChI=1S/C12H18O2/c1-9-4-6-12(7-5-9)10(2)8-14-11(3)13/h4,12H,2,5-8H2,1,3H3
InchiKey:	BCTDJPZNMXPMA-UHFFFAOYSA-N
Formula:	C12H18O2
SMILES:	<chem>C=C(COC(C)=O)C1CC=C(C)CC1</chem>
Mol. weight [g/mol]:	194.27
CAS:	15111-97-4

Physical Properties

Property code	Value	Unit	Source
gf	-59.69	kJ/mol	Joback Method
hf	-319.54	kJ/mol	Joback Method
hfus	19.70	kJ/mol	Joback Method
hvap	52.25	kJ/mol	Joback Method
log10ws	-3.07		Crippen Method
logp	2.852		Crippen Method
mcvol	167.920	ml/mol	McGowan Method
pc	2377.22	kPa	Joback Method
rinpol	1395.00		NIST Webbook
rinpol	1395.00		NIST Webbook
ripol	1846.00		NIST Webbook
ripol	1854.00		NIST Webbook
ripol	1856.00		NIST Webbook
ripol	1855.00		NIST Webbook
tb	570.50	K	Joback Method
tc	780.42	K	Joback Method
tf	302.10	K	Joback Method
vc	0.632	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	414.43	J/molxK	570.50	Joback Method
cpg	431.91	J/molxK	605.49	Joback Method
cpg	448.44	J/molxK	640.47	Joback Method
cpg	464.04	J/molxK	675.46	Joback Method
cpg	478.73	J/molxK	710.45	Joback Method
cpg	492.52	J/molxK	745.43	Joback Method
cpg	505.45	J/molxK	780.42	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C15111974&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
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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