

trans-Myrtanyl acetate

Inchi:	InChI=1S/C12H20O2/c1-8(13)14-7-9-4-5-10-6-11(9)12(10,2)3/h9-11H,4-7H2,1-3H3/t9-,1
InchiKey:	UWHRPSXEBAXLDR-HBNTYKKESA-N
Formula:	C12H20O2
SMILES:	CC(=O)OCC1CCC2CC1C2(C)C
Mol. weight [g/mol]:	196.29
CAS:	90934-53-5

Physical Properties

Property code	Value	Unit	Source
gf	-95.27	kJ/mol	Joback Method
hf	-421.81	kJ/mol	Joback Method
hfus	19.64	kJ/mol	Joback Method
hvap	49.69	kJ/mol	Joback Method
log10ws	-2.53		Crippen Method
logp	2.622		Crippen Method
mcvol	165.660	ml/mol	McGowan Method
pc	2356.49	kPa	Joback Method
rinpol	1381.00		NIST Webbook
rinpol	1381.00		NIST Webbook
rinpol	1360.00		NIST Webbook
rinpol	1381.00		NIST Webbook
rinpol	1379.00		NIST Webbook
rinpol	1379.00		NIST Webbook
ripol	1746.00		NIST Webbook
ripol	1746.00		NIST Webbook
tb	558.90	K	Joback Method
tc	766.28	K	Joback Method
tf	344.94	K	Joback Method
vc	0.633	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	438.95	J/mol×K	558.90	Joback Method

cpg	457.77	J/mol×K	593.46	Joback Method
cpg	475.48	J/mol×K	628.03	Joback Method
cpg	492.21	J/mol×K	662.59	Joback Method
cpg	508.06	J/mol×K	697.15	Joback Method
cpg	523.16	J/mol×K	731.72	Joback Method
cpg	537.62	J/mol×K	766.28	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C90934535&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
ripol:	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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