

Isoverbanol, acetate

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C12H20O2/c1-7-5-11(14-8(2)13)10-6-9(7)12(10,3)4/h7,9-11H,5-6H2,1-4H3

SJTUFGGNSOBU CB-UHFFFAOYSA-N

C12H20O2

CC(=O)OC1CC(C)C2CC1C2(C)C

196.29

Physical Properties

Property code	Value	Unit	Source
gf	-102.98	kJ/mol	Joback Method
hf	-442.15	kJ/mol	Joback Method
hfus	20.71	kJ/mol	Joback Method
hvap	49.38	kJ/mol	Joback Method
log10ws	-2.64		Crippen Method
logp	2.620		Crippen Method
mcvol	165.660	ml/mol	McGowan Method
pc	2282.77	kPa	Joback Method
rinpol	1310.00		NIST Webbook
rinpol	1296.00		NIST Webbook
rinpol	1296.00		NIST Webbook
rinpol	1296.00		NIST Webbook
tb	554.23	K	Joback Method
tc	761.49	K	Joback Method
tf	340.70	K	Joback Method
vc	0.632	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	439.79	J/mol×K	554.23	Joback Method
cpg	459.08	J/mol×K	588.77	Joback Method
cpg	477.26	J/mol×K	623.32	Joback Method
cpg	494.44	J/mol×K	657.86	Joback Method
cpg	510.73	J/mol×K	692.40	Joback Method
cpg	526.25	J/mol×K	726.95	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R130053&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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