neo-Isoverbanol, acetate

Inchi: 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
InchiKey: SJTUFGGNSOBUCB-UHFFFAOYSA-N
Formula: C12H20O2
SMILES: CC(=O)OC1CC(C)C2CC1C2(C)C
Mol. weight [g/mol]: 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	1318.00		NIST Webbook
rinpol	1318.00		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
cpg	541.10	J/mol×K	761.49	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R130102&Units=SI

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

Latest version available from:
https://www.chemeo.com/cid/70-996-9/neo-Isoverbanol-acetate.pdf
Generated by Cheméo on 2025-12-05 16:13:52.690842098 +0000 UTC m=+4699430.220882752.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.