10-epi-Italicen-12-yl acetate

Inchi: InChI=1S/C17H26O2/c1-11-7-8-17-12(2)5-6-14(17)16(4,15(17)9-11)10-19-13(3)18/h9,12
InchiKey: WEGYMQPVQUNDTQ-SRQBIAJPSA-N
Formula: C17H26O2
SMILES: CC(=O)OCC1(C)C2C=C(C)CCC23C(C)CCC13
Mol. weight [g/mol]: 262.39

Physical Properties

Property code	Value	Unit	Source
gf	10.32	kJ/mol	Joback Method
hf	-396.82	kJ/mol	Joback Method
hfus	23.16	kJ/mol	Joback Method
hvap	60.71	kJ/mol	Joback Method
log10ws	-4.13		Crippen Method
logp	3.958		Crippen Method
mcvol	220.950	ml/mol	McGowan Method
pc	1859.51	kPa	Joback Method
rinpol	1765.00		NIST Webbook
rinpol	1765.00		NIST Webbook
tb	688.69	K	Joback Method
tc	909.97	K	Joback Method
tf	452.89	K	Joback Method
vc	0.847	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	668.83	J/mol×K	688.69	Joback Method
cpg	689.94	J/mol×K	725.57	Joback Method
cpg	710.27	J/mol×K	762.45	Joback Method
cpg	730.07	J/mol×K	799.33	Joback Method
cpg	749.63	J/mol×K	836.21	Joback Method
cpg	769.19	J/mol×K	873.09	Joback Method
cpg	789.03	J/mol×K	909.97	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R232981&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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/60-740-3/10-epi-Italicen-12-yl-acetate.pdf

Generated by Cheméo on 2024-10-12 06:22:42.379015764 +0000 UTC m=+3295025.015985012.

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.