10-epi-«alpha»-Muurolol (T-Muurolol)

Inchi: InChI=1S/C15H28O/c1-10(2)12-7-8-15(4,16)14-6-5-11(3)9-13(12)14/h10-14,16H,5-9H2,1
InchiKey: RYSZDRWMTKGBFI-HONHCDKBSA-N
Formula: C15H28O
SMILES: CC1CCC2C(C1)C(C(C)C)CCC2(C)O
Mol. weight [g/mol]: 224.38

Physical Properties

Property code	Value	Unit	Source
gf	-19.36	kJ/mol	Joback Method
hf	-435.26	kJ/mol	Joback Method
hfus	19.96	kJ/mol	Joback Method
hvap	63.71	kJ/mol	Joback Method
log10ws	-4.06		Crippen Method
logp	3.856		Crippen Method
mcvol	206.360	ml/mol	McGowan Method
pc	1971.80	kPa	Joback Method
rinpol	1638.00		NIST Webbook
rinpol	1639.00		NIST Webbook
tb	651.13	K	Joback Method
tc	853.71	K	Joback Method
tf	337.61	K	Joback Method
vc	0.765	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	621.88	J/mol×K	651.13	Joback Method
cpg	643.47	J/mol×K	684.89	Joback Method
cpg	663.95	J/mol×K	718.66	Joback Method
cpg	683.44	J/mol×K	752.42	Joback Method
cpg	702.05	J/mol×K	786.19	Joback Method
cpg	719.88	J/mol×K	819.95	Joback Method
cpg	737.04	J/mol×K	853.71	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=R229420&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