«tau»-Muurolol

Other names:	4-Isopropyl-1,6-dimethyl-1,2,3,4,4a,7,8,8a-octahydro-1-naphthalenol-, [1S-(1«alpha»,4«alpha»,4a«alpha»,8a«alpha»)]- «alpha»-epi-Muurolol epi-«alpha»-Muurolol Muurolol T T-Muurolol 10-epi-«alpha»-Muurolol (-)-T-Muurolol T-Muurolol t-muurulol epi- «alpha»-Muurulol epi-«alpha»-Muurol T-Muurolol (10-epi-«alpha»-muurolol) T-Muurolol (epi-«alpha»-muurolol) epi-«alpha»-Muurolol («tau»-Muurolol)
Inchi:	InChI=1S/C15H26O/c1-10(2)12-7-8-15(4,16)14-6-5-11(3)9-13(12)14/h9-10,12-14,16H,5-
InchiKey:	LHYHMMRYTDARSZ-KBUPBQIOSA-N
Formula:	C15H26O
SMILES:	CC1=CC2C(C(C)C)CCC(C)(O)C2CC1
Mol. weight [g/mol]:	222.37
CAS:	19912-62-0

Physical Properties

Property code	Value	Unit	Source
gf	8.68	kJ/mol	Joback Method
hf	-368.61	kJ/mol	Joback Method
hfus	19.72	kJ/mol	Joback Method
hvap	64.97	kJ/mol	Joback Method
log10ws	-4.15		Crippen Method
logp	3.776		Crippen Method
mcvol	202.060	ml/mol	McGowan Method
pc	2069.88	kPa	Joback Method
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tb	659.94	K	Joback Method
tc	865.11	K	Joback Method
tf	355.13	K	Joback Method
vc	0.752	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	597.80	J/mol×K	659.94	Joback Method
cpg	617.79	J/mol×K	694.13	Joback Method
cpg	636.77	J/mol×K	728.33	Joback Method
cpg	654.86	J/mol×K	762.52	Joback Method
cpg	672.18	J/mol×K	796.72	Joback Method
cpg	688.83	J/mol×K	830.91	Joback Method
cpg	704.93	J/mol×K	865.11	Joback Method

Sources

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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

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

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