

«alpha»-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-YJNKXOJESA-N

Formula:

C15H26O

SMILES:

CC1=CC2C(C(C)C)CCC(C)(O)C2CC1

Mol. weight [g/mol]:

222.37

Physical Properties

Property code	Value	Unit	Source
hf	-285.47	kJ/mol	Cheméo Relay (1.0)
hfus	19.72	kJ/mol	Joback Method
hvap	82.40	kJ/mol	Cheméo Relay (1.0)
ie	8.36	eV	Cheméo Relay (1.0)
logp	3.776		Crippen Method
mcvol	202.060	ml/mol	McGowan Method
rinpol	1648.00		NIST Webbook
rinpol	1630.00		NIST Webbook
rinpol	1630.00		NIST Webbook
rinpol	1645.00		NIST Webbook
rinpol	1652.00		NIST Webbook
rinpol	1654.00		NIST Webbook
rinpol	1646.00		NIST Webbook
rinpol	1646.00		NIST Webbook
rinpol	1630.00		NIST Webbook
rinpol	1618.00		NIST Webbook
rinpol	1649.00		NIST Webbook
rinpol	1646.00		NIST Webbook
rinpol	1643.00		NIST Webbook
rinpol	1646.00		NIST Webbook
rinpol	1647.00		NIST Webbook
rinpol	1649.00		NIST Webbook
rinpol	1643.00		NIST Webbook
rinpol	1646.00		NIST Webbook
rinpol	1649.00		NIST Webbook
rinpol	1646.00		NIST Webbook
rinpol	1646.00		NIST Webbook
tb	557.65	K	Cheméo Relay (1.0)

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

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R603437&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature

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