

14-Hydroxy-«alpha»-muurolene

Other names:	«alpha»-Muurolene-14-ol «alpha»-Muurolene-14-hydroxy
Inchi:	InChI=1S/C15H24O/c1-10(2)13-6-4-11(3)14-7-5-12(9-16)8-15(13)14/h4,8,10,13-16H,5-7
InchiKey:	DFIKBBWSGFHYMP-UHFFFAOYSA-N
Formula:	C15H24O
SMILES:	CC1=CC2C(CC1)C(C)=CCC2C(C)CO
Mol. weight [g/mol]:	220.35
CAS:	135118-51-3

Physical Properties

Property code	Value	Unit	Source
gf	42.21	kJ/mol	Joback Method
hf	-317.20	kJ/mol	Joback Method
hfus	25.78	kJ/mol	Joback Method
hvap	67.39	kJ/mol	Joback Method
log10ws	-3.89		Crippen Method
logp	3.554		Crippen Method
mcvol	197.760	ml/mol	McGowan Method
pc	2086.93	kPa	Joback Method
rinpol	1780.00		NIST Webbook
rinpol	1757.00		NIST Webbook
rinpol	1775.00		NIST Webbook
rinpol	1777.00		NIST Webbook
rinpol	1775.00		NIST Webbook
rinpol	1780.00		NIST Webbook
rinpol	1782.20		NIST Webbook
rinpol	1775.00		NIST Webbook
rinpol	1756.00		NIST Webbook
rinpol	1777.00		NIST Webbook
rinpol	1775.00		NIST Webbook
rinpol	1770.00		NIST Webbook
rinpol	1782.20		NIST Webbook
rinpol	1780.00		NIST Webbook
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rinpol	1775.00		NIST Webbook
rinpol	1775.00		NIST Webbook
rinpol	1781.00		NIST Webbook

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rinpol	1776.00		NIST Webbook
rinpol	1780.00		NIST Webbook
rinpol	1782.00		NIST Webbook
rinpol	1757.00		NIST Webbook
rinpol	1764.00		NIST Webbook
rinpol	1788.00		NIST Webbook
rinpol	1780.00		NIST Webbook
rinpol	1772.00		NIST Webbook
rinpol	1783.00		NIST Webbook
rinpol	1780.00		NIST Webbook
ripol	2599.00		NIST Webbook
ripol	2567.00		NIST Webbook
ripol	2599.00		NIST Webbook
ripol	2599.00		NIST Webbook
tb	668.51	K	Joback Method
tc	869.60	K	Joback Method
tf	348.75	K	Joback Method
vc	0.742	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	576.51	J/mol×K	668.51	Joback Method
cpg	594.95	J/mol×K	702.02	Joback Method
cpg	612.33	J/mol×K	735.54	Joback Method
cpg	628.69	J/mol×K	769.05	Joback Method
cpg	644.06	J/mol×K	802.57	Joback Method
cpg	658.50	J/mol×K	836.08	Joback Method
cpg	672.04	J/mol×K	869.60	Joback Method
dvisc	0.0048013	Pa×s	348.75	Joback Method
dvisc	0.0016816	Pa×s	402.04	Joback Method
dvisc	0.0007529	Pa×s	455.34	Joback Method
dvisc	0.0003989	Pa×s	508.63	Joback Method
dvisc	0.0002384	Pa×s	561.92	Joback Method
dvisc	0.0001558	Pa×s	615.22	Joback Method
dvisc	0.0001089	Pa×s	668.51	Joback Method

Sources

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=C135118513&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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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