

«alpha»-Muurolene

Other names:	[1«alpha»,4a«alpha»,8a«alpha»]-1,2,4a,5,6,8a-hexahydro-4-7-dimethyl-1-[1-methylethyl]Naphthalene, 1,2,4a,5,6,8a-hexahydro-4,7-dimethyl-1-(1-methylethyl)-, (1«alpha»,4a«alpha»,8a«alpha»)-1«xi»,6«xi»,7«xi»-Cadina-4,9-diene 1-Isopropyl-4,7-dimethyl-1,2,4a,5,6,8a-hexahydronaphthalene, (1«alpha»,4a«alpha»,8a«alpha»)-Naphthalene, 1,2,4a,5,6,8a-hexahydro-4,7-dimethyl-1-(1-methylethyl)-, (1R,4aR,8aS)-rel-Muurolene
Inchi:	InChI=1S/C15H24/c1-10(2)13-8-6-12(4)14-7-5-11(3)9-15(13)14/h6,9-10,13-15H,5,7-8H2
InchiKey:	QMAYBMKBYCGXDH-ZNMIVQPWSA-N
Formula:	C15H24
SMILES:	CC1=CC2C(CC1)C(C)=CCC2C(C)C
Mol. weight [g/mol]:	204.35
CAS:	31983-22-9

Physical Properties

Property code	Value	Unit	Source
gf	179.03	kJ/mol	Joback Method
hf	-164.97	kJ/mol	Joback Method
hfus	21.69	kJ/mol	Joback Method
hvap	50.71	kJ/mol	Joback Method
log10ws	-4.63		Crippen Method
logp	4.581		Crippen Method
mcvol	191.890	ml/mol	McGowan Method
pc	1921.98	kPa	Joback Method
tb	576.33	K	Joback Method
tc	791.72	K	Joback Method
tf	287.93	K	Joback Method
vc	0.723	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	503.29	J/mol×K	576.33	Joback Method
cpg	526.08	J/mol×K	612.23	Joback Method
cpg	547.54	J/mol×K	648.13	Joback Method

cpg	567.74	J/mol×K	684.03	Joback Method
cpg	586.71	J/mol×K	719.93	Joback Method
cpg	604.51	J/mol×K	755.83	Joback Method
cpg	621.19	J/mol×K	791.72	Joback Method
dvisc	0.0020754	Pa×s	287.93	Joback Method
dvisc	0.0012375	Pa×s	336.00	Joback Method
dvisc	0.0008398	Pa×s	384.06	Joback Method
dvisc	0.0006213	Pa×s	432.13	Joback Method
dvisc	0.0004882	Pa×s	480.20	Joback Method
dvisc	0.0004008	Pa×s	528.26	Joback Method
dvisc	0.0003401	Pa×s	576.33	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C31983229&Units=SI

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

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