

«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»-Cadiña-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
mccvol	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	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	503.29	J/mol×K	576.33	Joback Method
cpg	604.51	J/mol×K	755.83	Joback Method
cpg	586.71	J/mol×K	719.93	Joback Method

cpg	567.74	J/molxK	684.03	Joback Method
cpg	547.54	J/molxK	648.13	Joback Method
cpg	526.08	J/molxK	612.23	Joback Method
cpg	621.19	J/molxK	791.72	Joback Method
dvisc	0.0003401	Paxs	576.33	Joback Method
dvisc	0.0004008	Paxs	528.26	Joback Method
dvisc	0.0004882	Paxs	480.20	Joback Method
dvisc	0.0006213	Paxs	432.13	Joback Method
dvisc	0.0008398	Paxs	384.06	Joback Method
dvisc	0.0012375	Paxs	336.00	Joback Method
dvisc	0.0020754	Paxs	287.93	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=C31983229&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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