

muurola-4,11-diene

Inchi:	InChI=1S/C15H24/c1-10(2)13-8-6-12(4)14-7-5-11(3)9-15(13)14/h11-12,14H,1,5-9H2,2-4
InchiKey:	BDGCRWMOCSWZSC-UHFFFAOYSA-N
Formula:	C15H24
SMILES:	C=C(C)C1=C2CC(C)CCC2C(C)CC1
Mol. weight [g/mol]:	204.35

Physical Properties

Property code	Value	Unit	Source
gf	230.80	kJ/mol	Joback Method
hf	-101.83	kJ/mol	Joback Method
hfus	21.40	kJ/mol	Joback Method
hvap	50.22	kJ/mol	Joback Method
log10ws	-4.87		Crippen Method
logp	4.725		Crippen Method
mcvol	191.890	ml/mol	McGowan Method
pc	1927.05	kPa	Joback Method
ripol	1457.00		NIST Webbook
ripol	1467.00		NIST Webbook
ripol	1457.00		NIST Webbook
ripol	1457.00		NIST Webbook
ripol	1467.00		NIST Webbook
ripol	1645.00		NIST Webbook
ripol	1629.00		NIST Webbook
ripol	1674.00		NIST Webbook
ripol	1646.00		NIST Webbook
ripol	1674.00		NIST Webbook
tb	574.17	K	Joback Method
tc	791.30	K	Joback Method
tf	286.45	K	Joback Method
vc	0.725	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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cpg	501.80	J/mol×K	574.17	Joback Method
cpg	525.03	J/mol×K	610.36	Joback Method
cpg	546.90	J/mol×K	646.55	Joback Method
cpg	567.47	J/mol×K	682.74	Joback Method
cpg	586.78	J/mol×K	718.92	Joback Method
cpg	604.90	J/mol×K	755.11	Joback Method
cpg	621.88	J/mol×K	791.30	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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=R233726&Units=SI

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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