

Valerena-4,7(11)-diene

Inchi:	InChI=1S/C15H24/c1-10(2)9-13-7-5-11(3)14-8-6-12(4)15(13)14/h9,11,13-14H,5-8H2,1-4H
InchiKey:	MZZFDMZYIBWOOA-UHFFFAOYSA-N
Formula:	C15H24
SMILES:	CC(C)=CC1CCC(C)C2CCC(C)=C12
Mol. weight [g/mol]:	204.35
CAS:	351222-66-7

Physical Properties

Property code	Value	Unit	Source
gf	235.28	kJ/mol	Joback Method
hf	-103.88	kJ/mol	Joback Method
hfus	24.98	kJ/mol	Joback Method
hvap	50.67	kJ/mol	Joback Method
log10ws	-4.87		Crippen Method
logp	4.725		Crippen Method
mcvol	191.890	ml/mol	McGowan Method
pc	1901.92	kPa	Joback Method
rinpol	1455.40		NIST Webbook
rinpol	1465.30		NIST Webbook
rinpol	1465.30		NIST Webbook
rinpol	1456.00		NIST Webbook
tb	577.38	K	Joback Method
tc	792.00	K	Joback Method
tf	286.65	K	Joback Method
vc	0.732	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	502.26	J/mol×K	577.38	Joback Method
cpg	524.59	J/mol×K	613.15	Joback Method
cpg	545.60	J/mol×K	648.92	Joback Method
cpg	565.37	J/mol×K	684.69	Joback Method
cpg	583.96	J/mol×K	720.46	Joback Method

cpg	601.44	J/mol×K	756.23	Joback Method
cpg	617.88	J/mol×K	792.00	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=C351222667&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

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

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