

(E)2,(Z)4,(E)6-ALLOFARNESENE

Inchi:	InChI=1S/C15H24/c1-6-14(4)10-8-12-15(5)11-7-9-13(2)3/h6,8-10,12H,7,11H2,1-5H3/b10
InchiKey:	JEKGHHPMLRLCIW-NSURDWQSSA-N
Formula:	C15H24
SMILES:	CC=C(C)C=CC=C(C)CCC=C(C)C
Mol. weight [g/mol]:	204.35

Physical Properties

Property code	Value	Unit	Source
gf	370.65	kJ/mol	Joback Method
hf	86.58	kJ/mol	Joback Method
hfus	31.48	kJ/mol	Joback Method
hvap	49.06	kJ/mol	Joback Method
log10ws	-5.52		Crippen Method
logp	5.202		Crippen Method
mcvol	205.010	ml/mol	McGowan Method
pc	1686.56	kPa	Joback Method
ripol	1631.00		NIST Webbook
ripol	1631.00		NIST Webbook
ripol	1932.00		NIST Webbook
ripol	1932.00		NIST Webbook
ripol	1932.00		NIST Webbook
tb	558.88	K	Joback Method
tc	753.82	K	Joback Method
tf	196.61	K	Joback Method
vc	0.798	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	485.53	J/molxK	558.88	Joback Method
cpg	503.84	J/molxK	591.37	Joback Method
cpg	521.10	J/molxK	623.86	Joback Method
cpg	537.41	J/molxK	656.35	Joback Method
cpg	552.83	J/molxK	688.84	Joback Method

cpg	567.43	J/mol×K	721.33	Joback Method
cpg	581.30	J/mol×K	753.82	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=R234516&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
rinpola:	Non-polar retention indices
ripola:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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