

(E)-Caryophyllene

Inchi: InChI=1S/C15H24/c1-11-6-5-7-12(2)13-10-15(3,4)14(13)9-8-11/h6,13-14H,2,5,7-10H2,1,
InchiKey: NPNUFJAVOONJE-IOMPXFEGSA-N
Formula: C15H24
SMILES: C=C1CCC=C(C)CCC2C1CC2(C)C
Mol. weight [g/mol]: 204.35

Physical Properties

Property code	Value	Unit	Source
gf	196.63	kJ/mol	Joback Method
hf	-112.68	kJ/mol	Joback Method
hfus	14.82	kJ/mol	Joback Method
hvap	49.32	kJ/mol	Joback Method
log10ws	-4.87		Crippen Method
logp	4.725		Crippen Method
mcvol	191.890	ml/mol	McGowan Method
pc	2027.23	kPa	Joback Method
rinpol	1411.00		NIST Webbook
rinpol	1423.00		NIST Webbook
rinpol	1420.00		NIST Webbook
rinpol	1411.00		NIST Webbook
rinpol	1424.00		NIST Webbook
rinpol	1420.00		NIST Webbook
rinpol	1420.00		NIST Webbook
rinpol	1418.00		NIST Webbook
rinpol	1416.00		NIST Webbook
rinpol	1415.00		NIST Webbook
rinpol	1423.00		NIST Webbook
rinpol	1433.00		NIST Webbook
rinpol	1418.00		NIST Webbook
rinpol	1418.00		NIST Webbook
rinpol	1421.00		NIST Webbook
rinpol	1419.00		NIST Webbook
rinpol	1420.00		NIST Webbook
rinpol	1419.00		NIST Webbook
rinpol	1424.00		NIST Webbook
rinpol	1411.00		NIST Webbook
rinpol	1418.00		NIST Webbook

ripol	1419.00		NIST Webbook
ripol	1419.00		NIST Webbook
ripol	1411.00		NIST Webbook
ripol	1564.00		NIST Webbook
ripol	1564.00		NIST Webbook
ripol	1598.00		NIST Webbook
ripol	1612.00		NIST Webbook
tb	576.30	K	Joback Method
tc	802.06	K	Joback Method
tf	323.71	K	Joback Method
vc	0.717	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	501.77	J/mol×K	576.30	Joback Method
cpg	525.28	J/mol×K	613.93	Joback Method
cpg	547.37	J/mol×K	651.55	Joback Method
cpg	568.18	J/mol×K	689.18	Joback Method
cpg	587.84	J/mol×K	726.81	Joback Method
cpg	606.51	J/mol×K	764.43	Joback Method
cpg	624.31	J/mol×K	802.06	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=R603442&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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