

(E,E)-7,11,15-Trimethyl-3-methylene-hexadeca-1,6

Other names:	«beta»-Springene
Inchi:	InChI=1S/C20H32/c1-7-18(4)12-9-14-20(6)16-10-15-19(5)13-8-11-17(2)3/h7,11,14-15H,1
InchiKey:	XSIVJVJUIXOEPW-YTOAGJIJSA-N
Formula:	C20H32
SMILES:	C=CC(=C)CCC=C(C)CCC=C(C)CCC=C(C)C
Mol. weight [g/mol]:	272.47
CAS:	70901-63-2

Physical Properties

Property code	Value	Unit	Source
gf	499.66	kJ/mol	Joback Method
hf	107.23	kJ/mol	Joback Method
hfus	40.36	kJ/mol	Joback Method
hvap	58.97	kJ/mol	Joback Method
log10ws	-7.46		Crippen Method
logp	6.928		Crippen Method
mcvol	271.160	ml/mol	McGowan Method
pc	1207.31	kPa	Joback Method
tb	662.36	K	Joback Method
tc	849.12	K	Joback Method
tf	240.56	K	Joback Method
vc	1.062	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	729.57	J/mol×K	662.36	Joback Method
cpg	749.24	J/mol×K	693.49	Joback Method
cpg	767.91	J/mol×K	724.61	Joback Method
cpg	785.66	J/mol×K	755.74	Joback Method
cpg	802.56	J/mol×K	786.86	Joback Method
cpg	818.67	J/mol×K	817.99	Joback Method
cpg	834.09	J/mol×K	849.12	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C70901632&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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

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