

(E,E)-7,11,15-TRIMETHYL-3-METHYLENE-HEXADIENE

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,1,2,4,6,8,10,12,13,16,17,18,19,20H
InchiKey:	XSIVJVJUIXOEPW-YTOAGJIJSA-N
Formula:	C20H32
SMILES:	C=CC(=C)CC/C=C(\C)CC/C=C(\C)CCC=C(C)C
Mol. weight [g/mol]:	272.48

Physical Properties

Property code	Value	Unit	Source
hf	-21.57	kJ/mol	Cheméo Relay (1.0)
hfus	40.36	kJ/mol	Joback Method
hvap	86.11	kJ/mol	Cheméo Relay (1.0)
log10ws	-6.76		Cheméo Relay (1.0)
logp	6.928		Crippen Method
mcvol	271.160	ml/mol	McGowan Method
tb	583.08	K	Cheméo Relay (1.0)
tf	235.51	K	Cheméo Relay (1.0)

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

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C70901632&Units=SI

Legend

cpg:	Ideal gas heat capacity
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
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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