(E,E,E)-3,7,11,15-Tetramethylhexadeca-1,3,6,10,14

Other names:	(3E,6E,10E)-3,7,11,15-Tetramethyl-1,3,6,10,14-hexadecapentaene
	(E,E,E)- «alpha»-Springene
	«alpha»-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/h7,11-12,14-15
InchiKey:	KFHRKQVLZRJWNB-OBHWEXPVSA-N
Formula:	C20H32
SMILES:	C=CC(C)=CCC=C(C)CCC=C(C)CCC=C(C)C
Mol. weight [g/mol]:	272.47
CAS:	77898-97-6

Physical Properties

Property code	Value	Unit	Source
gf	492.04	kJ/mol	Joback Method
hf	99.02	kJ/mol	Joback Method
hfus	41.84	kJ/mol	Joback Method
hvap	59.60	kJ/mol	Joback Method
log10ws	-7.46		Crippen Method
logp	6.928		Crippen Method
mcvol	271.160	ml/mol	McGowan Method
pc	1215.74	kPa	Joback Method
rinpol	1969.10		NIST Webbook
rinpol	2013.00		NIST Webbook
rinpol	2019.00		NIST Webbook
tb	669.84	K	Joback Method
tc	860.07	K	Joback Method
tf	237.24	K	Joback Method
vc	1.060	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	731.70	J/mol×K	669.84	Joback Method
cpg	751.44	J/mol×K	701.55	Joback Method
cpg	770.17	J/mol×K	733.25	Joback Method

cpg	787.96	J/mol×K	764.96	Joback Method
cpg	804.92	J/mol×K	796.66	Joback Method
cpg	821.11	J/mol×K	828.37	Joback Method
cpg	836.63	J/mol×K	860.07	Joback Method

Sources

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=C77898976&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

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