

(S,E)-8,12,15,15-Tetramethyl-4-methylenebicyclo[9

Inchi:

lnchl=1S/C20H32/c1-15-7-6-8-16(2)10-14-19-17(3)11-13-18(12-9-15)20(19,4)5/h8,18H,1

InchiKey:

SNPPNYAGNBWZCL-XSZFBFBBSA-N

Formula:

C20H32

SMILES:

C=C1CCC=C(C)CCC2=C(C)CCC(CC1)C2(C)C

Mol. weight [g/mol]:

272.47

CAS:

386223-19-4

Physical Properties

Property code	Value	Unit	Source
gf	208.74	kJ/mol	Joback Method
hf	-185.34	kJ/mol	Joback Method
hfus	18.75	kJ/mol	Joback Method
hvap	63.07	kJ/mol	Joback Method
log10ws	-7.06		Crippen Method
logp	6.596		Crippen Method
mcvol	258.040	ml/mol	McGowan Method
pc	1523.50	kPa	Joback Method
rinpol	2026.80		NIST Webbook
tb	721.57	K	Joback Method
tc	958.52	K	Joback Method
tf	396.02	K	Joback Method
vc	0.952	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	771.97	J/mol×K	721.57	Joback Method
cpg	798.29	J/mol×K	761.06	Joback Method
cpg	823.12	J/mol×K	800.55	Joback Method
cpg	846.58	J/mol×K	840.04	Joback Method
cpg	868.80	J/mol×K	879.54	Joback Method
cpg	889.92	J/mol×K	919.03	Joback Method
cpg	910.07	J/mol×K	958.52	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C386223194&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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