1H-Trindene, 2,3,4,5,6,7,8,9-octahydro-1,1,4,4,9,9-hexamethyl-

Inchi: InChI=1S/C21H30/c1-19(2)10-7-13-14-8-11-20(3,4)17(14)18-15(16(13)19)9-12-21(18,5)6

InchiKey: PYBVWXXGQXNHDK-UHFFFAOYSA-N

Formula: C21H30

SMILES: CC1(C)CCc2c3c(c4c(c21)CCC4(C)C)C(C)(C)CC3

Mol. weight [g/mol]: 282.46

CAS: 55682-87-6

Physical Properties

Property code	Value	Unit	Source
gf	355.98	kJ/mol	Joback Method
hf	-33.47	kJ/mol	Joback Method
hfus	17.75	kJ/mol	Joback Method
hvap	64.21	kJ/mol	Joback Method
log10ws	-6.25		Crippen Method
logp	5.358		Crippen Method
mcvol	250.410	ml/mol	McGowan Method
pc	1661.90	kPa	Joback Method
tb	752.40	K	Joback Method
tc	990.72	K	Joback Method
tf	382.00 ± 4.00	K	NIST Webbook
vc	0.969	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	768.50	J/mol×K	752.40	Joback Method
cpg	791.84	J/mol×K	792.12	Joback Method
cpg	815.46	J/mol×K	831.84	Joback Method
cpg	839.88	J/mol×K	871.56	Joback Method
cpg	865.59	J/mol×K	911.28	Joback Method
cpg	893.08	J/mol×K	951.00	Joback Method
cpg	922.87	J/mol×K	990.72	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C55682876&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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