

7-Isopropyl-1,1,4a-trimethyl-1,2,3,4,4a,9,10,10a-oc

Inchi:	InChI=1S/C20H30/c1-14(2)15-7-9-17-16(13-15)8-10-18-19(3,4)11-6-12-20(17,18)5/h7,9,
InchiKey:	QUUCYKKMFLJLFS-UHFFFAOYSA-N
Formula:	C20H30
SMILES:	CC(C)c1ccc2c(c1)CCC1C(C)(C)CCCC21C
Mol. weight [g/mol]:	270.45
CAS:	109680-01-5

Physical Properties

Property code	Value	Unit	Source
gf	286.84	kJ/mol	Joback Method
hf	-104.40	kJ/mol	Joback Method
hfus	17.84	kJ/mol	Joback Method
hvap	60.89	kJ/mol	Joback Method
log10ws	-6.17		Crippen Method
logp	5.840		Crippen Method
mcvol	247.180	ml/mol	McGowan Method
pc	1649.77	kPa	Joback Method
rinpol	2073.90		NIST Webbook
tb	711.03	K	Joback Method
tc	947.41	K	Joback Method
tf	424.02	K	Joback Method
vc	0.934	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	740.09	J/molxK	711.03	Joback Method
cpg	764.29	J/molxK	750.43	Joback Method
cpg	787.63	J/molxK	789.82	Joback Method
cpg	810.45	J/molxK	829.22	Joback Method
cpg	833.07	J/molxK	868.62	Joback Method
cpg	855.84	J/molxK	908.01	Joback Method
cpg	879.08	J/molxK	947.41	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=C109680015&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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
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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