

1,1,4,7-Tetramethyl-1a,2,3,4,6,7,7a,7b-octahydro-1

Inchi:	InChI=1S/C15H24/c1-9-6-8-12-14(15(12,3)4)13-10(2)5-7-11(9)13/h7,9-10,12-14H,5-6,8H
InchiKey:	KDDAGEWDPAMROQ-UHFFFAOYSA-N
Formula:	C15H24
SMILES:	CC1CCC2C(C3C1=CCC3C)C2(C)C
Mol. weight [g/mol]:	204.35
CAS:	405112-35-8

Physical Properties

Property code	Value	Unit	Source
gf	225.18	kJ/mol	Joback Method
hf	-146.32	kJ/mol	Joback Method
hfus	22.56	kJ/mol	Joback Method
hvap	47.94	kJ/mol	Joback Method
log10ws	-4.19		Crippen Method
logp	4.271		Crippen Method
mvol	185.330	ml/mol	McGowan Method
pc	1973.55	kPa	Joback Method
rinpol	1446.80		NIST Webbook
rinpol	1446.80		NIST Webbook
tb	561.73	K	Joback Method
tc	778.35	K	Joback Method
tf	330.05	K	Joback Method
vc	0.712	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	505.21	J/molxK	561.73	Joback Method
cpg	528.79	J/molxK	597.83	Joback Method
cpg	550.88	J/molxK	633.94	Joback Method
cpg	571.64	J/molxK	670.04	Joback Method
cpg	591.24	J/molxK	706.14	Joback Method
cpg	609.85	J/molxK	742.24	Joback Method
cpg	627.64	J/molxK	778.35	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C405112358&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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