

4,11,11-trimethyl-8-methylenebicyclo[7.2.0]undecane

Inchi:

lnchl=1S/C15H24/c1-11-6-5-7-12(2)13-10-15(3,4)14(13)9-8-11/h8,13-14H,2,5-7,9-10H2

InchiKey:

NSMRKFBAPAOVQL-DHZHZOJOSA-N

Formula:

C15H24

SMILES:

C=C1CCCC(C)=CCC2C1CC2(C)C

Mol. weight [g/mol]:

204.35

CAS:

889360-49-0

Physical Properties

Property code	Value	Unit	Source
gf	196.63	kJ/mol	Joback Method
hf	-112.68	kJ/mol	Joback Method
hfus	14.82	kJ/mol	Joback Method
hvap	49.32	kJ/mol	Joback Method
log10ws	-4.87		Crippen Method
logp	4.725		Crippen Method
mcvol	191.890	ml/mol	McGowan Method
pc	2027.23	kPa	Joback Method
rinpol	1460.20		NIST Webbook
tb	576.30	K	Joback Method
tc	802.06	K	Joback Method
tf	323.71	K	Joback Method
vc	0.717	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	501.77	J/mol×K	576.30	Joback Method
cpg	525.28	J/mol×K	613.93	Joback Method
cpg	547.37	J/mol×K	651.55	Joback Method
cpg	568.18	J/mol×K	689.18	Joback Method
cpg	587.84	J/mol×K	726.81	Joback Method
cpg	606.51	J/mol×K	764.43	Joback Method
cpg	624.31	J/mol×K	802.06	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=C889360490&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
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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