

Sibirene

Inchi:	InChI=1S/C15H24/c1-11(2)13-7-9-15(4)8-5-6-12(3)14(15)10-13/h10-11,13H,3,5-9H2,1-2
InchiKey:	MBANDXQCQFFUAJ-AWKYBWMHSA-N
Formula:	C15H24
SMILES:	<chem>C=C1CCCC2(C)CCC(C(C)C)C=C12</chem>
Mol. weight [g/mol]:	204.35

Physical Properties

Property code	Value	Unit	Source
gf	214.00	kJ/mol	Joback Method
hf	-91.46	kJ/mol	Joback Method
hfus	12.33	kJ/mol	Joback Method
hvap	49.07	kJ/mol	Joback Method
log10ws	-4.87		Crippen Method
logp	4.725		Crippen Method
mcvol	191.890	ml/mol	McGowan Method
pc	2056.76	kPa	Joback Method
rinpol	1400.00		NIST Webbook
rinpol	1394.00		NIST Webbook
rinpol	1400.00		NIST Webbook
rinpol	1399.00		NIST Webbook
rinpol	1394.00		NIST Webbook
tb	576.26	K	Joback Method
tc	799.10	K	Joback Method
tf	316.47	K	Joback Method
vc	0.720	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	499.60	J/molxK	576.26	Joback Method
cpg	522.01	J/molxK	613.40	Joback Method
cpg	543.03	J/molxK	650.54	Joback Method
cpg	562.83	J/molxK	687.68	Joback Method
cpg	581.54	J/molxK	724.82	Joback Method

cpg	599.33	J/mol×K	761.96	Joback Method
cpg	616.34	J/mol×K	799.10	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=R610747&Units=SI

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
hvac:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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