

sibirene

Inchi:	InChI=1S/C15H24/c1-11(2)13-7-9-15(4)8-5-6-12(3)14(15)10-13/h10-11,14H,3,5-9H2,1-2
InchiKey:	MBANDXQCQFFUAJ-AWKYBWMHSA-N
Formula:	C15H24
SMILES:	C=C1CCC[C@@]2(C)CCC(C(C)C)=CC12
Mol. weight [g/mol]:	204.36

Physical Properties

Property code	Value	Unit	Source
hfus	12.33	kJ/mol	Joback Method
logp	4.725		Crippen Method
mcpvol	191.890	ml/mol	McGowan Method

Temperature Dependent Properties

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

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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<https://www.chemeo.com/cid/75-064-8/sibirene.pdf>

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