

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:	ALUIZDJKPCNAGJ-YSSOQSIOSA-N
Formula:	C15H24
SMILES:	<chem>C=C1CCCC2(C)CCC(C(C)C)=CC12</chem>
Mol. weight [g/mol]:	204.35
CAS:	14029-18-6

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	1426.70		NIST Webbook
rinpol	1458.00		NIST Webbook
rinpol	1457.70		NIST Webbook
rinpol	1426.70		NIST Webbook
ripol	1594.00		NIST Webbook
ripol	1594.00		NIST Webbook
ripol	1594.00		NIST Webbook
tb	576.26	K	Joback Method
tc	799.10	K	Joback Method
tf	316.47	K	Joback Method
vc	0.720	m ³ /kmol	Joback 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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C14029186&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
ripola:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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