

epi-Bicyclosesqjuiphellandrene

Inchi:	InChI=1S/C15H24/c1-10(2)13-8-6-12(4)14-7-5-11(3)9-15(13)14/h9-10,12-14H,3,5-8H2,1
InchiKey:	RNDFUOKDULDZPR-AMIUJLCOSA-N
Formula:	C15H24
SMILES:	<chem>C=C1C=C2C(C(C)C)CCC(C)C2CC1</chem>
Mol. weight [g/mol]:	204.35

Physical Properties

Property code	Value	Unit	Source
gf	211.78	kJ/mol	Joback Method
hf	-127.04	kJ/mol	Joback Method
hfus	19.70	kJ/mol	Joback Method
hvap	49.91	kJ/mol	Joback Method
log10ws	-4.63		Crippen Method
logp	4.581		Crippen Method
mcvol	191.890	ml/mol	McGowan Method
pc	1918.62	kPa	Joback Method
rinqol	1435.00		NIST Webbook
tb	571.35	K	Joback Method
tc	785.53	K	Joback Method
tf	288.33	K	Joback Method
vc	0.721	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	501.64	J/molxK	571.35	Joback Method
cpg	524.63	J/molxK	607.05	Joback Method
cpg	546.31	J/molxK	642.74	Joback Method
cpg	566.71	J/molxK	678.44	Joback Method
cpg	585.88	J/molxK	714.14	Joback Method
cpg	603.88	J/molxK	749.83	Joback Method
cpg	620.74	J/molxK	785.53	Joback Method
dvisc	0.0022043	Paxs	288.33	Joback Method
dvisc	0.0013305	Paxs	335.50	Joback Method

dvisc	0.0009095	Paxs	382.67	Joback Method
dvisc	0.0006759	Paxs	429.84	Joback Method
dvisc	0.0005326	Paxs	477.01	Joback Method
dvisc	0.0004381	Paxs	524.18	Joback Method
dvisc	0.0003722	Paxs	571.35	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R642343&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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
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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