

(+)**epi-Bicyclosquesquiphellandrene**

Other names:	Bicyclosquesquiphellandrene
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-UHFFFAOYSA-N
Formula:	C15H24
SMILES:	<chem>C=C1C=C2C(C(C)C)CCC(C)C2CC1</chem>
Mol. weight [g/mol]:	204.35
CAS:	54324-03-7

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
rinpol	1490.00		NIST Webbook
rinpol	1471.00		NIST Webbook
rinpol	1488.00		NIST Webbook
rinpol	1521.00		NIST Webbook
rinpol	1481.00		NIST Webbook
rinpol	1490.00		NIST Webbook
rinpol	1489.00		NIST Webbook
rinpol	1489.00		NIST Webbook
rinpol	1498.70		NIST Webbook
rinpol	1470.00		NIST Webbook
rinpol	1489.00		NIST Webbook
rinpol	1498.70		NIST Webbook
rinpol	1493.00		NIST Webbook
rinpol	1491.00		NIST Webbook
rinpol	1495.00		NIST Webbook
rinpol	1488.00		NIST Webbook
ripol	1748.00		NIST Webbook
ripol	1706.00		NIST Webbook
ripol	1760.00		NIST Webbook

ripol	1760.00		NIST Webbook
ripol	1760.00		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/mol×K	571.35	Joback Method
cpg	524.63	J/mol×K	607.05	Joback Method
cpg	546.31	J/mol×K	642.74	Joback Method
cpg	566.71	J/mol×K	678.44	Joback Method
cpg	585.88	J/mol×K	714.14	Joback Method
cpg	603.88	J/mol×K	749.83	Joback Method
cpg	620.74	J/mol×K	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

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=C54324037&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

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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
ripol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:

<https://www.cheméo.com/cid/76-157-4/epi-Bicyclosesquiphellandrene.pdf>

Generated by Cheméo on 2024-04-20 14:06:20.386701061 +0000 UTC m=+15911229.307278374.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.