

Bicycloelemene

Inchi:

InChI=1S/C15H24/c1-7-15(6)9-8-11-13(14(11,4)5)12(15)10(2)3/h7,11-13H,1-2,8-9H2,3-6H2

InchiKey:

LKQMMFFQYMYQOJ-COMQUAJESA-N

Formula:

C15H24

SMILES:

C=CC1(C)CCC2C(C1C(=C)C)C2(C)C

Mol. weight [g/mol]:

204.35

CAS:

32531-56-9

Physical Properties

Property code	Value	Unit	Source
gf	317.84	kJ/mol	Joback Method
hf	-2.96	kJ/mol	Joback Method
hfus	15.52	kJ/mol	Joback Method
hvap	44.49	kJ/mol	Joback Method
log10ws	-4.39		Crippen Method
logp	4.437		Crippen Method
mcvol	191.890	ml/mol	McGowan Method
pc	1901.92	kPa	Joback Method
rinpol	1338.00		NIST Webbook
rinpol	1338.00		NIST Webbook
rinpol	1335.00		NIST Webbook
rinpol	1330.00		NIST Webbook
rinpol	1336.00		NIST Webbook
rinpol	1338.00		NIST Webbook
rinpol	1334.00		NIST Webbook
rinpol	1335.00		NIST Webbook
rinpol	1341.00		NIST Webbook
rinpol	1326.00		NIST Webbook
rinpol	1346.00		NIST Webbook
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ripol	1481.00		NIST Webbook
ripol	1478.00		NIST Webbook
ripol	1471.00		NIST Webbook
ripol	1481.00		NIST Webbook
ripol	1495.00		NIST Webbook
ripol	1495.00		NIST Webbook
ripol	1484.00		NIST Webbook
tb	540.06	K	Joback Method
tc	751.89	K	Joback Method
tf	308.77	K	Joback Method
vc	0.738	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	493.03	J/mol×K	540.06	Joback Method
cpg	515.30	J/mol×K	575.36	Joback Method
cpg	536.06	J/mol×K	610.67	Joback Method
cpg	555.54	J/mol×K	645.97	Joback Method
cpg	573.97	J/mol×K	681.28	Joback Method
cpg	591.59	J/mol×K	716.58	Joback Method
cpg	608.63	J/mol×K	751.89	Joback Method

Sources

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C32531569&Units=SI>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307I>

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
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
rnpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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