

1,10-di-epi-Cubenol

Other names:	1-10-epi-Cubenol Cubenol (1,10 di-epi) Cubenol (1,10 di-epi-)
Inchi:	InChI=1S/C15H26O/c1-10(2)13-6-5-12(4)15(16)8-7-11(3)9-14(13)15/h9-10,12-14,16H,5-
InchiKey:	COGPRPSWSKCLKTF-NZATWWQASA-N
Formula:	C15H26O
SMILES:	CC1=CC2C(C(C)C)CCC(C)C2(O)CC1
Mol. weight [g/mol]:	222.37
CAS:	73365-77-2

Physical Properties

Property code	Value	Unit	Source
gf	8.68	kJ/mol	Joback Method
hf	-368.61	kJ/mol	Joback Method
hfus	19.72	kJ/mol	Joback Method
hvap	64.97	kJ/mol	Joback Method
log10ws	-4.15		Crippen Method
logp	3.776		Crippen Method
mcvol	202.060	ml/mol	McGowan Method
pc	2069.88	kPa	Joback Method
rinpol	1612.00		NIST Webbook
rinpol	1613.00		NIST Webbook
rinpol	1613.00		NIST Webbook
rinpol	1616.00		NIST Webbook
rinpol	1590.00		NIST Webbook
rinpol	1607.00		NIST Webbook
rinpol	1612.00		NIST Webbook
rinpol	1602.00		NIST Webbook
rinpol	1619.00		NIST Webbook
rinpol	1610.00		NIST Webbook
rinpol	1617.00		NIST Webbook
rinpol	1614.00		NIST Webbook
rinpol	1617.00		NIST Webbook
rinpol	1614.00		NIST Webbook
rinpol	1614.00		NIST Webbook
rinpol	1607.00		NIST Webbook
rinpol	1616.00		NIST Webbook

rinpol	1599.00	NIST Webbook
rinpol	1636.20	NIST Webbook
rinpol	1618.00	NIST Webbook
rinpol	1589.00	NIST Webbook
rinpol	1618.00	NIST Webbook
rinpol	1612.00	NIST Webbook
rinpol	1623.00	NIST Webbook
rinpol	1618.00	NIST Webbook
rinpol	1610.00	NIST Webbook
rinpol	1610.00	NIST Webbook
rinpol	1625.00	NIST Webbook
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rinpol	1618.00	NIST Webbook
rinpol	1619.00	NIST Webbook
rinpol	1618.00	NIST Webbook
rinpol	1612.00	NIST Webbook
ripol	2037.00	NIST Webbook
ripol	2022.00	NIST Webbook
ripol	2054.00	NIST Webbook
ripol	2054.00	NIST Webbook
ripol	2057.00	NIST Webbook
ripol	2054.00	NIST Webbook
ripol	2056.00	NIST Webbook
ripol	2037.00	NIST Webbook
ripol	2074.00	NIST Webbook

tb	659.94	K	Joback Method
tc	865.11	K	Joback Method
tf	355.13	K	Joback Method
vc	0.752	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	597.80	J/mol×K	659.94	Joback Method
cpg	617.79	J/mol×K	694.13	Joback Method
cpg	636.77	J/mol×K	728.33	Joback Method
cpg	654.86	J/mol×K	762.52	Joback Method
cpg	672.18	J/mol×K	796.72	Joback Method
cpg	688.83	J/mol×K	830.91	Joback Method
cpg	704.93	J/mol×K	865.11	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=C73365772&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

rinpol:	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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