

«beta»-Copaen-4-ol

Inchi:	InChI=1S/C15H24O/c1-8(2)10-5-6-15(4)11-7-12(16)9(3)14(15)13(10)11/h8,10-14,16H,3,
InchiKey:	LPXOPRGPLUWGKB-VXLSKKRHS-A-N
Formula:	C15H24O
SMILES:	C=C1C(O)CC2C3C(C(C)C)CCC2(C)C13
Mol. weight [g/mol]:	220.35

Physical Properties

Property code	Value	Unit	Source
gf	130.77	kJ/mol	Joback Method
hf	-259.74	kJ/mol	Joback Method
hfus	23.23	kJ/mol	Joback Method
hvap	63.27	kJ/mol	Joback Method
log10ws	-3.56		Crippen Method
logp	3.242		Crippen Method
mcvol	191.200	ml/mol	McGowan Method
pc	2108.07	kPa	Joback Method
rinpol	1566.00		NIST Webbook
rinpol	1574.00		NIST Webbook
rinpol	1574.00		NIST Webbook
rinpol	1585.00		NIST Webbook
rinpol	1584.00		NIST Webbook
rinpol	1566.00		NIST Webbook
rinpol	1584.00		NIST Webbook
tb	644.22	K	Joback Method
tc	842.77	K	Joback Method
tf	379.79	K	Joback Method
vc	0.731	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	576.73	J/mol×K	644.22	Joback Method
cpg	595.44	J/mol×K	677.31	Joback Method
cpg	613.20	J/mol×K	710.40	Joback Method

cpg	630.15	J/mol×K	743.49	Joback Method
cpg	646.41	J/mol×K	776.58	Joback Method
cpg	662.12	J/mol×K	809.68	Joback Method
cpg	677.43	J/mol×K	842.77	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R324446&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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

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