

«beta»-Copaen-4-«alpha»-ol

Other names:	«beta»-Copaene-4«alpha»-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-UHFFFAOYSA-N
Formula:	C15H24O
SMILES:	C=C1C(O)CC2C3C(C(C)C)CCC2(C)C13
Mol. weight [g/mol]:	220.35
CAS:	124753-76-0

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	1587.00		NIST Webbook
rinpol	1583.00		NIST Webbook
rinpol	1579.00		NIST Webbook
rinpol	1585.00		NIST Webbook
rinpol	1570.00		NIST Webbook
rinpol	1565.00		NIST Webbook
rinpol	1575.00		NIST Webbook
rinpol	1579.00		NIST Webbook
rinpol	1570.00		NIST Webbook
rinpol	1565.00		NIST Webbook
rinpol	1596.30		NIST Webbook
rinpol	1595.00		NIST Webbook
rinpol	1585.00		NIST Webbook
rinpol	1572.00		NIST Webbook
rinpol	1579.00		NIST Webbook
rinpol	1590.00		NIST Webbook
rinpol	1587.00		NIST Webbook
rinpol	1589.00		NIST Webbook
rinpol	1594.00		NIST Webbook

rinpol	1589.00		NIST Webbook
rinpol	1588.00		NIST Webbook
rinpol	1586.00		NIST Webbook
rinpol	1572.00		NIST Webbook
rinpol	1586.00		NIST Webbook
rinpol	1581.00		NIST Webbook
rinpol	1575.00		NIST Webbook
rinpol	1586.00		NIST Webbook
rinpol	1575.00		NIST Webbook
rinpol	1595.00		NIST Webbook
rinpol	1591.00		NIST Webbook
rinpol	1584.00		NIST Webbook
rinpol	1556.00		NIST Webbook
rinpol	1595.00		NIST Webbook
rinpol	1584.00		NIST Webbook
rinpol	1586.00		NIST Webbook
rinpol	1596.30		NIST Webbook
rinpol	1585.00		NIST Webbook
rinpol	1591.00		NIST Webbook
ripol	2141.00		NIST Webbook
ripol	2135.00		NIST Webbook
ripol	2141.00		NIST Webbook
ripol	2135.00		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

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C124753760&Units=SI

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

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