

«alpha»-Copaen-8-ol

Inchi:	InChI=1S/C15H24O/c1-9(2)15(16)8-7-14(4)11-6-5-10(3)12(14)13(11)15/h5,9,11-13,16H,
InchiKey:	OHKRJLLHVVS RK-KLDMJIFRSA-N
Formula:	C15H24O
SMILES:	CC1=CCC2C3C1C2(C)CCC3(O)C(C)C
Mol. weight [g/mol]:	220.35

Physical Properties

Property code	Value	Unit	Source
gf	100.24	kJ/mol	Joback Method
hf	-262.09	kJ/mol	Joback Method
hfus	17.86	kJ/mol	Joback Method
hvap	63.22	kJ/mol	Joback Method
log10ws	-3.81		Crippen Method
logp	3.386		Crippen Method
mcvol	191.200	ml/mol	McGowan Method
pc	2271.90	kPa	Joback Method
rinpol	1626.00		NIST Webbook
rinpol	1590.00		NIST Webbook
rinpol	1605.00		NIST Webbook
rinpol	1590.00		NIST Webbook
ripol	2123.00		NIST Webbook
ripol	2082.00		NIST Webbook
tb	654.11	K	Joback Method
tc	860.54	K	Joback Method
tf	407.53	K	Joback Method
vc	0.732	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	572.53	J/mol×K	654.11	Joback Method
cpg	590.51	J/mol×K	688.52	Joback Method
cpg	607.71	J/mol×K	722.92	Joback Method
cpg	624.38	J/mol×K	757.33	Joback Method

cpg	640.76	J/mol×K	791.73	Joback Method
cpg	657.07	J/mol×K	826.14	Joback Method
cpg	673.56	J/mol×K	860.54	Joback Method

Sources

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=R320266&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

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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