

5-Hydroxycalamenene

Inchi:	InChI=1S/C15H22O/c1-9(2)12-6-5-11(4)15-13(12)7-10(3)8-14(15)16/h7-9,11-12,16H,5-6
InchiKey:	FDMKIGKOMRSCAW-NEPJUHHUSA-N
Formula:	C15H22O
SMILES:	<chem>Cc1cc(O)c2c(c1)C(C(C)C)CCC2C</chem>
Mol. weight [g/mol]:	218.33
CAS:	95908-33-1

Physical Properties

Property code	Value	Unit	Source
gf	52.45	kJ/mol	Joback Method
hf	-275.63	kJ/mol	Joback Method
hfus	27.24	kJ/mol	Joback Method
hvap	64.99	kJ/mol	Joback Method
log10ws	-4.36		Crippen Method
logp	4.338		Crippen Method
mcvol	193.460	ml/mol	McGowan Method
pc	2315.84	kPa	Joback Method
rinpol	2068.00		NIST Webbook
rinpol	2068.00		NIST Webbook
ripol	2325.00		NIST Webbook
ripol	2325.00		NIST Webbook
tb	665.76	K	Joback Method
tc	893.47	K	Joback Method
tf	417.17	K	Joback Method
vc	0.675	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	547.17	J/molxK	665.76	Joback Method
cpg	629.78	J/molxK	855.52	Joback Method
cpg	615.14	J/molxK	817.56	Joback Method
cpg	599.66	J/molxK	779.61	Joback Method
cpg	583.24	J/molxK	741.66	Joback Method

cpg	565.78	J/molxK	703.71	Joback Method
cpg	643.69	J/molxK	893.47	Joback Method
dvisc	0.0000379	Paxs	665.76	Joback Method
dvisc	0.0000546	Paxs	624.33	Joback Method
dvisc	0.0000827	Paxs	582.90	Joback Method
dvisc	0.0001337	Paxs	541.47	Joback Method
dvisc	0.0002338	Paxs	500.03	Joback Method
dvisc	0.0004524	Paxs	458.60	Joback Method
dvisc	0.0009983	Paxs	417.17	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C95908331&Units=SI
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

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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

Latest version available from:

<https://www.chemeo.com/cid/79-019-4/5-Hydroxycalamenene.pdf>

Generated by Cheméo on 2024-04-23 16:55:51.093125945 +0000 UTC m=+16180600.013703262.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.