

10-Hydroxycalamenene

Inchi:	InChI=1S/C15H22O/c1-10(2)13-6-4-11(3)14-7-5-12(9-16)8-15(13)14/h5,7-8,10-11,13,16
InchiKey:	LXEZVXMZNFZNA-UHFFFAOYSA-N
Formula:	C15H22O
SMILES:	CC1CCC(C(C)C)c2cc(CO)ccc21
Mol. weight [g/mol]:	218.33

Physical Properties

Property code	Value	Unit	Source
gf	70.25	kJ/mol	Joback Method
hf	-250.55	kJ/mol	Joback Method
hfus	25.54	kJ/mol	Joback Method
hvap	68.65	kJ/mol	Joback Method
log10ws	-4.47		Crippen Method
logp	3.816		Crippen Method
mcvol	193.460	ml/mol	McGowan Method
pc	2193.84	kPa	Joback Method
rinpol	1645.00		NIST Webbook
rinpol	1653.00		NIST Webbook
rinpol	1645.00		NIST Webbook
ripol	2390.00		NIST Webbook
tb	677.32	K	Joback Method
tc	880.91	K	Joback Method
tf	366.27	K	Joback Method
vc	0.729	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	550.83	J/molxK	677.32	Joback Method
cpg	567.70	J/molxK	711.25	Joback Method
cpg	583.59	J/molxK	745.18	Joback Method
cpg	598.53	J/molxK	779.11	Joback Method
cpg	612.58	J/molxK	813.04	Joback Method
cpg	625.78	J/molxK	846.98	Joback Method

cpg	638.18	J/molxK	880.91	Joback Method
dvisc	0.0033634	Paxs	366.27	Joback Method
dvisc	0.0012769	Paxs	418.11	Joback Method
dvisc	0.0006003	Paxs	469.95	Joback Method
dvisc	0.0003278	Paxs	521.80	Joback Method
dvisc	0.0001997	Paxs	573.64	Joback Method
dvisc	0.0001321	Paxs	625.48	Joback Method
dvisc	0.0000931	Paxs	677.32	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=R198311&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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

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