

1,2-Dehydroglobulol

Inchi:	InChI=1S/C15H24O/c1-9-5-6-10-12(9)13-11(14(13,2)3)7-8-15(10,4)16/h6,9,11-13,16H,5
InchiKey:	RMMXVRYYNCFLLS-ADRMSITKSA-N
Formula:	C15H24O
SMILES:	CC1CC=C2C1C1C(CCC2(C)O)C1(C)C
Mol. weight [g/mol]:	220.35

Physical Properties

Property code	Value	Unit	Source
gf	82.87	kJ/mol	Joback Method
hf	-283.31	kJ/mol	Joback Method
hfus	20.35	kJ/mol	Joback Method
hvap	63.47	kJ/mol	Joback Method
log10ws	-3.81		Crippen Method
logp	3.386		Crippen Method
mcvol	191.200	ml/mol	McGowan Method
pc	2237.64	kPa	Joback Method
ripol	1524.00		NIST Webbook
ripol	1561.00		NIST Webbook
ripol	1524.00		NIST Webbook
ripol	2115.00		NIST Webbook
ripol	2115.00		NIST Webbook
tb	654.15	K	Joback Method
tc	862.88	K	Joback Method
tf	414.77	K	Joback Method
vc	0.729	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	576.39	J/molxK	654.15	Joback Method
cpg	595.29	J/molxK	688.94	Joback Method
cpg	613.37	J/molxK	723.73	Joback Method
cpg	630.87	J/molxK	758.52	Joback Method
cpg	648.01	J/molxK	793.31	Joback Method

cpg	665.02	J/mol×K	828.10	Joback Method
cpg	682.13	J/mol×K	862.88	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R228665&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

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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