

Chiloscyphone

Inchi:	InChI=1S/C15H22O/c1-9(2)12-7-5-10(3)13-8-6-11(4)15(16)14(12)13/h5,9,12-14H,4,6-8H
InchiKey:	VDMHNWBQSSGYNR-UHFFFAOYSA-N
Formula:	C15H22O
SMILES:	<chem>C=C1CCC2C(C)=CCC(C(C)C)C2C1=O</chem>
Mol. weight [g/mol]:	218.33
CAS:	23538-45-6

Physical Properties

Property code	Value	Unit	Source
gf	89.19	kJ/mol	Joback Method
hf	-264.74	kJ/mol	Joback Method
hfus	19.21	kJ/mol	Joback Method
hvap	54.16	kJ/mol	Joback Method
log10ws	-3.91		Crippen Method
logp	3.760		Crippen Method
mcvol	193.460	ml/mol	McGowan Method
pc	1978.82	kPa	Joback Method
tb	639.17	K	Joback Method
tc	866.07	K	Joback Method
tf	356.55	K	Joback Method
vc	0.728	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	543.23	J/molxK	639.17	Joback Method
cpg	565.16	J/molxK	676.99	Joback Method
cpg	585.76	J/molxK	714.80	Joback Method
cpg	605.04	J/molxK	752.62	Joback Method
cpg	623.01	J/molxK	790.44	Joback Method
cpg	639.71	J/molxK	828.25	Joback Method
cpg	655.13	J/molxK	866.07	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=C23538456&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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