

Shyobunol

Other names:	Schyobunol
Inchi:	InChI=1S/C15H26O/c1-7-15(6)9-8-12(10(2)3)14(16)13(15)11(4)5/h7,10,12-14,16H,1,4,8
InchiKey:	WOULTTPZJDSDEI-UHFFFAOYSA-N
Formula:	C15H26O
SMILES:	<chem>C=CC1(C)CCC(C(C)C)C(O)C1C(=C)C</chem>
Mol. weight [g/mol]:	222.37
CAS:	35727-45-8

Physical Properties

Property code	Value	Unit	Source
gf	99.12	kJ/mol	Joback Method
hf	-260.83	kJ/mol	Joback Method
hfus	20.05	kJ/mol	Joback Method
hvap	62.37	kJ/mol	Joback Method
log10ws	-4.11		Crippen Method
logp	3.798		Crippen Method
mcvol	208.620	ml/mol	McGowan Method
pc	1861.11	kPa	Joback Method
ripol	1701.00		NIST Webbook
ripol	1721.00		NIST Webbook
ripol	1709.00		NIST Webbook
ripol	1701.00		NIST Webbook
ripol	1689.00		NIST Webbook
ripol	1687.00		NIST Webbook
ripol	1687.00		NIST Webbook
ripol	1697.00		NIST Webbook
ripol	1953.00		NIST Webbook
ripol	1953.00		NIST Webbook
ripol	1953.00		NIST Webbook
ripol	1953.00		NIST Webbook
ripol	1930.00		NIST Webbook
tb	633.36	K	Joback Method
tc	827.92	K	Joback Method
tf	305.71	K	Joback Method
vc	0.779	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	586.93	J/mol×K	633.36	Joback Method
cpg	606.35	J/mol×K	665.79	Joback Method
cpg	624.82	J/mol×K	698.21	Joback Method
cpg	642.44	J/mol×K	730.64	Joback Method
cpg	659.29	J/mol×K	763.06	Joback Method
cpg	675.46	J/mol×K	795.49	Joback Method
cpg	691.04	J/mol×K	827.92	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C35727458&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
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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