

Shiromool

Inchi:	InChI=1S/C15H26O2/c1-10(2)12-8-7-11(3)6-5-9-15(4)14(17-15)13(12)16/h6,10,12-14,16
InchiKey:	KLQPHHIQARFSDE-NCMQTQOKSA-N
Formula:	C15H26O2
SMILES:	CC1=CCCC2(C)OC2C(O)C(C(C)C)CC1
Mol. weight [g/mol]:	238.37
CAS:	28892-14-0

Physical Properties

Property code	Value	Unit	Source
gf	-89.54	kJ/mol	Joback Method
hf	-506.77	kJ/mol	Joback Method
hfus	25.60	kJ/mol	Joback Method
hvap	69.66	kJ/mol	Joback Method
log10ws	-3.95		Crippen Method
logp	3.297		Crippen Method
mvol	207.930	ml/mol	McGowan Method
pc	2100.34	kPa	Joback Method
rinpol	1810.00		NIST Webbook
tb	691.16	K	Joback Method
tc	900.77	K	Joback Method
tf	378.18	K	Joback Method
vc	0.765	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	635.64	J/molxK	691.16	Joback Method
cpg	655.63	J/molxK	726.09	Joback Method
cpg	674.61	J/molxK	761.03	Joback Method
cpg	692.71	J/molxK	795.96	Joback Method
cpg	710.04	J/molxK	830.90	Joback Method
cpg	726.71	J/molxK	865.83	Joback Method
cpg	742.83	J/molxK	900.77	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C28892140&Units=SI

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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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