

Turmerol

Inchi: InChI=1S/C15H24O/c1-11(2)9-15(16)10-13(4)14-7-5-12(3)6-8-14/h5,8-9,13,15-16H,6-7,1
InchiKey: AEQCSQRYHBNSGA-UHFFFAOYSA-N
Formula: C15H24O
SMILES: CC(C)=CC(O)CC(C)C1=CCC(C)=CC1
Mol. weight [g/mol]: 220.35

Physical Properties

Property code	Value	Unit	Source
gf	78.21	kJ/mol	Joback Method
hf	-241.01	kJ/mol	Joback Method
hfus	22.97	kJ/mol	Joback Method
hvap	67.57	kJ/mol	Joback Method
log10ws	-4.69		Crippen Method
logp	4.006		Crippen Method
mcvol	204.320	ml/mol	McGowan Method
pc	2041.91	kPa	Joback Method
rinpol	1577.00		NIST Webbook
tb	670.44	K	Joback Method
tc	867.98	K	Joback Method
tf	308.77	K	Joback Method
vc	0.769	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	562.58	J/molxK	670.44	Joback Method
cpg	579.06	J/molxK	703.36	Joback Method
cpg	594.62	J/molxK	736.29	Joback Method
cpg	609.32	J/molxK	769.21	Joback Method
cpg	623.18	J/molxK	802.14	Joback Method
cpg	636.27	J/molxK	835.06	Joback Method
cpg	648.63	J/molxK	867.98	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R224772&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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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