Vulgarol B

Inchi: InChI=1S/C15H24O/c1-9-8-10(16)12-13-11(9)15(12,4)7-5-6-14(13,2)3/h8,10-13,16H,5-7
InchiKey: XQPMEWZJPNAPBK-KPGIFEJMSA-N
Formula: C15H24O
SMILES: CC1=CC(O)C2C3C1C2(C)CCCC3(C)C
Mol. weight [g/mol]: 220.35

Physical Properties

Property code	Value	Unit	Source
hfus	20.35	kJ/mol	Joback Method
logp	3.386		Crippen Method
mcvol	191.200	ml/mol	McGowan Method
rinpol	1688.00		NIST Webbook
rinpol	1688.00		NIST Webbook
ripol	2368.00		NIST Webbook
ripol	2368.00		NIST Webbook

Temperature Dependent Properties

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

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R336508&Units=SI
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
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
ripol:	Polar retention indices