Epishiobunol

Other names: Epishiobunol
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: C=CC1(C)CCC(C(C)C)C(O)C1C(=C)C
Mol. weight [g/mol]: 222.37

Physical Properties

Property code	Value	Unit	Source
hfus	20.05	kJ/mol	Joback Method
logp	3.798		Crippen Method
mcvol	208.620	ml/mol	McGowan 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

Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C69350614&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume