epi-Torilenol

Inchi: InChI=1S/C15H24O/c1-8(2)12-10-7-15(4)11(16)6-5-9(3)14(15)13(10)12/h8,10-14,16H,3,
InchiKey: WVVFQZGQVPKOMT-LQCPYWFOSA-N
Formula: C15H24O
SMILES: C=C1CCC(O)C2(C)CC3C(C(C)C)C3C12
Mol. weight [g/mol]: 220.35

Physical Properties

Property code	Value	Unit	Source
gf	130.77	kJ/mol	Joback Method
hf	-259.74	kJ/mol	Joback Method
hfus	23.23	kJ/mol	Joback Method
hvap	63.27	kJ/mol	Joback Method
log10ws	-3.56		Crippen Method
logp	3.242		Crippen Method
mcvol	191.200	ml/mol	McGowan Method
pc	2108.07	kPa	Joback Method
rinpol	1546.00		NIST Webbook
tb	644.22	K	Joback Method
tc	842.77	K	Joback Method
tf	379.79	K	Joback Method
vc	0.731	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	576.73	J/mol×K	644.22	Joback Method
cpg	595.44	J/mol×K	677.31	Joback Method
cpg	613.20	J/mol×K	710.40	Joback Method
cpg	630.15	J/mol×K	743.49	Joback Method
cpg	646.41	J/mol×K	776.58	Joback Method
cpg	662.12	J/mol×K	809.68	Joback Method
cpg	677.43	J/mol×K	842.77	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R201239&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume