Scirpentriol

Inchi: InChI=1S/C15H22O5/c1-8-3-4-14(6-16)9(5-8)20-12-10(17)11(18)13(14,2)15(12)7-19-15/
InchiKey: PXEBOIUZEXXBGH-BAIQKSCASA-N
Formula: C15H22O5
SMILES: CC1=CC2OC3C(O)C(O)C(C)(C2(CO)CC1)C31CO1
Mol. weight [g/mol]: 282.33
CAS: 2270-41-9

Physical Properties

Property code	Value	Unit	Source
gf	-307.75	kJ/mol	Joback Method
hf	-763.73	kJ/mol	Joback Method
hfus	36.32	kJ/mol	Joback Method
hvap	104.61	kJ/mol	Joback Method
log10ws	-1.58		Crippen Method
logp	-0.017		Crippen Method
mcvol	203.820	ml/mol	McGowan Method
pc	3181.14	kPa	Joback Method
rinpol	2260.00		NIST Webbook
rinpol	2260.00		NIST Webbook
tb	899.39	K	Joback Method
tc	1109.71	K	Joback Method
tf	631.39	K	Joback Method
vc	0.763	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	754.41	J/mol×K	899.39	Joback Method
cpg	775.08	J/mol×K	934.44	Joback Method
cpg	797.38	J/mol×K	969.50	Joback Method
cpg	821.66	J/mol×K	1004.55	Joback Method
cpg	848.24	J/mol×K	1039.61	Joback Method
cpg	877.46	J/mol×K	1074.66	Joback Method
cpg	909.66	J/mol×K	1109.71	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2270419&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