2«beta»-hydroxy-6«beta»-methoxy-trans-decalin

Inchi: InChI=1S/C11H20O2/c1-13-11-5-3-8-6-10(12)4-2-9(8)7-11/h8-12H,2-7H2,1H3/t8?,9?,10-

InchiKey: TUXPVWASPKOLEG-JPPWEJMLSA-N

Formula: C11H20O2

SMILES: COC1CCC2CC(O)CCC2C1

Mol. weight [g/mol]: 184.28

Physical Properties

Property code	Value	Unit	Source
gf	-142.40	kJ/mol	Joback Method
hf	-474.54	kJ/mol	Joback Method
hfus	19.53	kJ/mol	Joback Method
hvap	59.06	kJ/mol	Joback Method
log10ws	-2.31		Crippen Method
logp	1.963		Crippen Method
mcvol	155.870	ml/mol	McGowan Method
pc	2755.56	kPa	Joback Method
rinpol	1484.00		NIST Webbook
rinpol	1484.00		NIST Webbook
ripol	2310.00		NIST Webbook
ripol	2310.00		NIST Webbook
tb	586.90	K	Joback Method
tc	788.20	K	Joback Method
tf	310.10	K	Joback Method
vc	0.569	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	436.40	J/mol×K	586.90	Joback Method
cpg	455.39	J/mol×K	620.45	Joback Method
cpg	473.36	J/mol×K	654.00	Joback Method
cpg	490.32	J/mol×K	687.55	Joback Method
cpg	506.29	J/mol×K	721.10	Joback Method
cpg	521.30	J/mol×K	754.65	Joback Method

cpg	535.37	J/mol×K	788.20	Joback Method
dvisc	0.0080384	Pa×s	310.10	Joback Method
dvisc	0.0028129	Pa×s	356.23	Joback Method
dvisc	0.0012523	Pa×s	402.37	Joback Method
dvisc	0.0006585	Pa×s	448.50	Joback Method
dvisc	0.0003904	Pa×s	494.63	Joback Method
dvisc	0.0002530	Pa×s	540.77	Joback Method
dvisc	0.0001756	Pa×s	586.90	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=R136279&Units=SI

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume