2«alpha»-hydroxy-6«alpha»-cyanide-trans-decalin

Inchi: InChI=1S/C11H17NO/c12-7-8-1-2-10-6-11(13)4-3-9(10)5-8/h8-11,13H,1-6H2/t8-,9?,10?,
InchiKey: NVYYORRRKLMLII-PMUOWJKOSA-N
Formula: C11H17NO
SMILES: N#CC1CCC2CC(O)CCC2C1
Mol. weight [g/mol]: 179.26

Physical Properties

Property code	Value	Unit	Source
gf	95.78	kJ/mol	Joback Method
hf	-177.44	kJ/mol	Joback Method
hfus	19.85	kJ/mol	Joback Method
hvap	67.13	kJ/mol	Joback Method
log10ws	-2.73		Crippen Method
logp	2.087		Crippen Method
mcvol	151.380	ml/mol	McGowan Method
pc	2732.56	kPa	Joback Method
rinpol	1588.00		NIST Webbook
ripol	2702.00		NIST Webbook
tb	666.56	K	Joback Method
tc	883.67	K	Joback Method
tf	352.86	K	Joback Method
vc	0.577	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	448.80	J/mol×K	666.56	Joback Method
cpg	465.08	J/mol×K	702.75	Joback Method
cpg	480.28	J/mol×K	738.93	Joback Method
cpg	494.45	J/mol×K	775.12	Joback Method
cpg	507.63	J/mol×K	811.30	Joback Method
cpg	519.86	J/mol×K	847.49	Joback Method
cpg	531.18	J/mol×K	883.67	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R136051&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume