2«alpha»-hydroxy-trans-decalin-6-one

Inchi: InChI=1S/C10H16O2/c11-9-3-1-7-5-10(12)4-2-8(7)6-9/h7-9,11H,1-6H2/t7?,8?,9-/m0/s1
InchiKey: GRGGRJRDSLLNJL-HACHORDNSA-N
Formula: C10H16O2
SMILES: O=C1CCC2CC(O)CCC2C1
Mol. weight [g/mol]: 168.23

Physical Properties

Property code	Value	Unit	Source
gf	-160.70	kJ/mol	Joback Method
hf	-439.04	kJ/mol	Joback Method
hfus	14.19	kJ/mol	Joback Method
hvap	58.98	kJ/mol	Joback Method
log10ws	-1.97		Crippen Method
logp	1.517		Crippen Method
mcvol	137.480	ml/mol	McGowan Method
pc	3364.54	kPa	Joback Method
rinpol	1503.00		NIST Webbook
rinpol	1503.00		NIST Webbook
ripol	2578.00		NIST Webbook
ripol	2578.00		NIST Webbook
tb	614.09	K	Joback Method
tc	833.81	K	Joback Method
tf	349.06	K	Joback Method
vc	0.502	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	391.23	J/mol×K	614.09	Joback Method
cpg	408.91	J/mol×K	650.71	Joback Method
cpg	425.53	J/mol×K	687.33	Joback Method
cpg	441.09	J/mol×K	723.95	Joback Method
cpg	455.62	J/mol×K	760.57	Joback Method
cpg	469.14	J/mol×K	797.19	Joback Method

cpg	481.65	J/mol×K	833.81	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=R136120&Units=SI

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