

2«alpha»-hydroxy-6«beta»-chloro-trans-decalin

Inchi:	InChI=1S/C10H17ClO/c11-9-3-1-8-6-10(12)4-2-7(8)5-9/h7-10,12H,1-6H2/t7?,8?,9-,10+/n
InchiKey:	RXFQKXWSWHBTLP-BMNUFHGDSA-N
Formula:	C10H17ClO
SMILES:	OC1CCC2CC(Cl)CCC2C1
Mol. weight [g/mol]:	188.69

Physical Properties

Property code	Value	Unit	Source
gf	-57.75	kJ/mol	Joback Method
hf	-337.42	kJ/mol	Joback Method
hfus	19.95	kJ/mol	Joback Method
hvap	58.81	kJ/mol	Joback Method
log10ws	-2.95		Crippen Method
logp	2.555		Crippen Method
mcvol	148.150	ml/mol	McGowan Method
pc	2989.32	kPa	Joback Method
ripol	1506.00		NIST Webbook
ripol	2398.00		NIST Webbook
ripol	2398.00		NIST Webbook
tb	579.03	K	Joback Method
tc	789.70	K	Joback Method
tf	306.52	K	Joback Method
vc	0.543	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	389.86	J/molxK	579.03	Joback Method
cpg	407.81	J/molxK	614.14	Joback Method
cpg	424.68	J/molxK	649.25	Joback Method
cpg	440.50	J/molxK	684.37	Joback Method
cpg	455.31	J/molxK	719.48	Joback Method
cpg	469.15	J/molxK	754.59	Joback Method
cpg	482.06	J/molxK	789.70	Joback Method

dvisc	0.0104547	Paxs	306.52	Joback Method
dvisc	0.0036965	Paxs	351.94	Joback Method
dvisc	0.0016576	Paxs	397.36	Joback Method
dvisc	0.0008763	Paxs	442.77	Joback Method
dvisc	0.0005216	Paxs	488.19	Joback Method
dvisc	0.0003391	Paxs	533.61	Joback Method
dvisc	0.0002359	Paxs	579.03	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R136086&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
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

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