

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

Inchi:	InChI=1S/C16H22O/c17-16-9-8-14-10-13(6-7-15(14)11-16)12-4-2-1-3-5-12/h1-5,13-17H,
InchiKey:	UYFIVGIKELBTNL-PRLABOORSA-N
Formula:	C16H22O
SMILES:	OC1CCC2CC(c3ccccc3)CCC2C1
Mol. weight [g/mol]:	230.35

Physical Properties

Property code	Value	Unit	Source
gf	117.11	kJ/mol	Joback Method
hf	-208.99	kJ/mol	Joback Method
hfus	25.34	kJ/mol	Joback Method
hvap	70.06	kJ/mol	Joback Method
log10ws	-4.27		Crippen Method
logp	3.731		Crippen Method
mcvol	196.690	ml/mol	McGowan Method
pc	2410.00	kPa	Joback Method
rinpol	1921.00		NIST Webbook
ripol	2944.00		NIST Webbook
tb	705.56	K	Joback Method
tc	931.90	K	Joback Method
tf	370.64	K	Joback Method
vc	0.723	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	602.02	J/molxK	705.56	Joback Method
cpg	622.32	J/molxK	743.28	Joback Method
cpg	641.13	J/molxK	781.01	Joback Method
cpg	658.53	J/molxK	818.73	Joback Method
cpg	674.59	J/molxK	856.45	Joback Method
cpg	689.40	J/molxK	894.17	Joback Method
cpg	703.01	J/molxK	931.90	Joback Method
dvisc	0.0045769	Paxs	370.64	Joback Method

dvisc	0.0016457	Paxs	426.46	Joback Method
dvisc	0.0007498	Paxs	482.28	Joback Method
dvisc	0.0004021	Paxs	538.10	Joback Method
dvisc	0.0002425	Paxs	593.92	Joback Method
dvisc	0.0001595	Paxs	649.74	Joback Method
dvisc	0.0001121	Paxs	705.56	Joback Method

Sources

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=R136284&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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