2«beta»-hydroxy-6«alpha»-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-SLTXQBBLSA-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	1919.00		NIST Webbook
rinpol	1919.00		NIST Webbook
ripol	2923.00		NIST Webbook
tb	705.56	K	Joback Method
tc	931.90	K	Joback Method
tf	370.64	K	Joback Method
vc	0.723	m3/kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0001121	Pa×s	705.56	Joback Method
dvisc	0.0001595	Pa×s	649.74	Joback Method
dvisc	0.0002425	Pa×s	593.92	Joback Method
dvisc	0.0004021	Pa×s	538.10	Joback Method
dvisc	0.0007498	Pa×s	482.28	Joback Method
dvisc	0.0016457	Pa×s	426.46	Joback Method
dvisc	0.0045769	Pa×s	370.64	Joback Method

Sources

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=R136224&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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