1-(Phenylmethylene)-1H-indene

Inchi: InChI=1S/C16H14/c1-2-6-13(7-3-1)12-15-11-10-14-8-4-5-9-16(14)15/h1-9,12H,10-11H2/
InchiKey: QTWIKOMWVWPBRX-NTCAYCPXSA-N
Formula: C16H14
SMILES: C(=C1CCc2ccccc21)c1ccccc1
Mol. weight [g/mol]: 206.28

Physical Properties

Property code	Value	Unit	Source
gf	412.95	kJ/mol	Joback Method
hf	257.19	kJ/mol	Joback Method
hfus	22.28	kJ/mol	Joback Method
hvap	57.43	kJ/mol	Joback Method
log10ws	-4.77		Crippen Method
logp	4.173		Crippen Method
mcvol	173.620	ml/mol	McGowan Method
pc	2726.86	kPa	Joback Method
rinpol	308.80		NIST Webbook
rinpol	308.80		NIST Webbook
tb	641.87	K	Joback Method
tc	897.34	K	Joback Method
tf	367.98	K	Joback Method
vc	0.656	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	433.27	J/mol×K	641.87	Joback Method
cpg	450.57	J/mol×K	684.45	Joback Method
cpg	466.42	J/mol×K	727.03	Joback Method
cpg	480.97	J/mol×K	769.61	Joback Method
cpg	494.37	J/mol×K	812.19	Joback Method
cpg	506.79	J/mol×K	854.76	Joback Method
cpg	518.37	J/mol×K	897.34	Joback Method
dvisc	0.0016108	Pa×s	367.98	Joback Method

dvisc	0.0010417	Pa×s	413.63	Joback Method
dvisc	0.0007346	Pa×s	459.28	Joback Method
dvisc	0.0005518	Pa×s	504.93	Joback Method
dvisc	0.0004347	Pa×s	550.57	Joback Method
dvisc	0.0003551	Pa×s	596.22	Joback Method
dvisc	0.0002986	Pa×s	641.87	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R411555&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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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