

2,2'-Biindanyl

Inchi:	InChI=1S/C18H18/c1-2-6-14-10-17(9-13(14)5-1)18-11-15-7-3-4-8-16(15)12-18/h1-8,17-1
InchiKey:	ICUGNAODJHKLQW-UHFFFAOYSA-N
Formula:	C18H18
SMILES:	<chem>c1ccc2c(c1)CC(C1Cc3ccccc3C1)C2</chem>
Mol. weight [g/mol]:	234.34
CAS:	39060-95-2

Physical Properties

Property code	Value	Unit	Source
gf	427.74	kJ/mol	Joback Method
hf	180.87	kJ/mol	Joback Method
hfus	25.95	kJ/mol	Joback Method
hvap	61.36	kJ/mol	Joback Method
log10ws	-4.80		Crippen Method
logp	3.816		Crippen Method
mvol	195.240	ml/mol	McGowan Method
pc	2370.28	kPa	Joback Method
tb	688.04	K	Joback Method
tc	943.03	K	Joback Method
tf	406.38	K	Joback Method
vc	0.742	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	547.56	J/mol×K	688.04	Joback Method
cpg	567.47	J/mol×K	730.54	Joback Method
cpg	585.79	J/mol×K	773.04	Joback Method
cpg	602.70	J/mol×K	815.54	Joback Method
cpg	618.38	J/mol×K	858.03	Joback Method
cpg	633.03	J/mol×K	900.53	Joback Method
cpg	646.83	J/mol×K	943.03	Joback Method
cpl	332.40	J/mol×K	298.15	NIST Webbook
dvisc	0.0022538	Paxs	406.38	Joback Method

dvisc	0.0017747	Paxs	453.32	Joback Method
dvisc	0.0014615	Paxs	500.27	Joback Method
dvisc	0.0012444	Paxs	547.21	Joback Method
dvisc	0.0010867	Paxs	594.15	Joback Method
dvisc	0.0009681	Paxs	641.10	Joback Method
dvisc	0.0008761	Paxs	688.04	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=C39060952&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
cpl:	Liquid phase 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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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