As-Indacene, 1,2,3,6,7,8-hexahydro-1,1,6,6-tetramethyl-4-(1-met

Other names: As-Hydrindacene, 4-isopropyl-1,1,6,6-tetramethyl-

Inchi: InChI=1S/C19H28/c1-12(2)15-11-16-14(8-9-18(16,3)4)17-13(15)7-10-19(17,5)6/h11-12H

InchiKey: BDVXGLCBHPSEGG-UHFFFAOYSA-N

Formula: C19H28

SMILES: CC(C)c1cc2c(c3c1CCC3(C)C)CCC2(C)C

Mol. weight [g/mol]: 256.43

CAS: 17465-47-3

Physical Properties

Property code	Value	Unit	Source
gf	291.07	kJ/mol	Joback Method
hf	-74.04	kJ/mol	Joback Method
hfus	17.60	kJ/mol	Joback Method
hvap	59.95	kJ/mol	Joback Method
log10ws	-5.84		Crippen Method
logp	5.258		Crippen Method
mcvol	233.090	ml/mol	McGowan Method
pc	1717.45	kPa	Joback Method
tb	694.24	K	Joback Method
tc	922.46	K	Joback Method
tf	355.00 ± 4.00	K	NIST Webbook
vc	0.895	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	674.63	J/mol×K	694.24	Joback Method
cpg	695.78	J/mol×K	732.28	Joback Method
cpg	716.27	J/mol×K	770.31	Joback Method
cpg	736.40	J/mol×K	808.35	Joback Method
cpg	756.50	J/mol×K	846.39	Joback Method
cpg	776.86	J/mol×K	884.42	Joback Method
cpg	797.79	J/mol×K	922.46	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C17465473&Units=SI

Legend

cpg:	Ideal gas heat capacity
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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