1,8-Dihydro-as-indacene

Inchi: InChI=1S/C12H10/c1-3-9-7-8-10-4-2-6-12(10)11(9)5-1/h1-3,5-7H,4,8H2
InchiKey: LHBLJJVZXVGWMH-UHFFFAOYSA-N
Formula: C12H10
SMILES: C1=CC2=CCC3=C(C=CC3)C2=C1
Mol. weight [g/mol]: 154.21
CAS: 18837-46-2

Physical Properties

Property code	Value	Unit	Source
gf	330.52	kJ/mol	Joback Method
hf	212.95	kJ/mol	Joback Method
hfus	16.28	kJ/mol	Joback Method
hvap	47.60	kJ/mol	Joback Method
log10ws	-3.80		Crippen Method
logp	3.069		Crippen Method
mcvol	125.860	ml/mol	McGowan Method
pc	3517.91	kPa	Joback Method
rinpol	255.10		NIST Webbook
rinpol	255.00		NIST Webbook
tb	536.72	K	Joback Method
tc	777.86	K	Joback Method
tf	334.86	K	Joback Method
vc	0.487	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	280.00	J/mol×K	536.72	Joback Method
cpg	294.23	J/mol×K	576.91	Joback Method
cpg	307.22	J/mol×K	617.10	Joback Method
cpg	319.10	J/mol×K	657.29	Joback Method
cpg	329.99	J/mol×K	697.48	Joback Method
cpg	340.05	J/mol×K	737.67	Joback Method
cpg	349.39	J/mol×K	777.86	Joback Method

dvisc	0.0014227	Pa×s	334.86	Joback Method
dvisc	0.0012105	Pa×s	368.50	Joback Method
dvisc	0.0010583	Pa×s	402.15	Joback Method
dvisc	0.0009445	Pa×s	435.79	Joback Method
dvisc	0.0008569	Pa×s	469.43	Joback Method
dvisc	0.0007876	Pa×s	503.08	Joback Method
dvisc	0.0007316	Pa×s	536.72	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C18837462&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