

9H-Indeno[1,2-e]pyrene

Inchi:	InChI=1S/C23H14/c1-2-8-17-16(5-1)13-20-18-9-3-6-14-11-12-15-7-4-10-19(23(17)20)22
InchiKey:	SIFHTIHFPPIGBL-UHFFFAOYSA-N
Formula:	C23H14
SMILES:	c1ccc2c(c1)Cc1c-2c2cccc3ccc4cccc1c4c32
Mol. weight [g/mol]:	290.36
CAS:	87308-65-4

Physical Properties

Property code	Value	Unit	Source
gf	726.30	kJ/mol	Joback Method
hf	530.87	kJ/mol	Joback Method
hfus	36.76	kJ/mol	Joback Method
hvap	78.82	kJ/mol	Joback Method
log10ws	-9.25		Crippen Method
logp	6.155		Crippen Method
mcvol	222.470	ml/mol	McGowan Method
pc	2318.07	kPa	Joback Method
tb	856.01	K	Joback Method
tc	1121.31	K	Joback Method
tf	598.01	K	Joback Method
vc	0.877	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	631.13	J/mol×K	856.01	Joback Method
cpg	645.60	J/mol×K	900.23	Joback Method
cpg	660.02	J/mol×K	944.44	Joback Method
cpg	674.72	J/mol×K	988.66	Joback Method
cpg	690.07	J/mol×K	1032.88	Joback Method
cpg	706.40	J/mol×K	1077.10	Joback Method
cpg	724.08	J/mol×K	1121.31	Joback Method
dvisc	0.0066224	Pa×s	598.01	Joback Method
dvisc	0.0063545	Pa×s	641.01	Joback Method

dvisc	0.0061292	Pa×s	684.01	Joback Method
dvisc	0.0059371	Pa×s	727.01	Joback Method
dvisc	0.0057716	Pa×s	770.01	Joback Method
dvisc	0.0056275	Pa×s	813.01	Joback Method
dvisc	0.0055010	Pa×s	856.01	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C87308654&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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