

11H-Indeno[2,1,7-cde]pyrene

Inchi:	InChI=1S/C21H12/c1-3-12-7-8-13-9-10-15-11-14-4-2-6-17-16(5-1)18(12)20(13)21(15)19
InchiKey:	IRMHVODPYNKKAP-UHFFFAOYSA-N
Formula:	C21H12
SMILES:	<chem>c1cc2c3c(c1)c1cccc4ccc5ccc(c3c5c41)C2</chem>
Mol. weight [g/mol]:	264.32
CAS:	59004-71-6

Physical Properties

Property code	Value	Unit	Source
gf	703.70	kJ/mol	Joback Method
hf	526.69	kJ/mol	Joback Method
hfus	34.56	kJ/mol	Joback Method
hvap	73.73	kJ/mol	Joback Method
log10ws	-8.45		Crippen Method
logp	5.641		Crippen Method
mcvol	198.590	ml/mol	McGowan Method
pc	2574.11	kPa	Joback Method
rinpol	474.21		NIST Webbook
rinpol	474.21		NIST Webbook
tb	802.55	K	Joback Method
tc	1062.21	K	Joback Method
tf	581.75	K	Joback Method
vc	0.795	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	543.75	J/mol×K	802.55	Joback Method
cpg	556.52	J/mol×K	845.83	Joback Method
cpg	569.14	J/mol×K	889.10	Joback Method
cpg	581.94	J/mol×K	932.38	Joback Method
cpg	595.27	J/mol×K	975.65	Joback Method
cpg	609.49	J/mol×K	1018.93	Joback Method
cpg	624.92	J/mol×K	1062.21	Joback Method

dvisc	0.0102272	Paxs	581.75	Joback Method
dvisc	0.0103866	Paxs	618.55	Joback Method
dvisc	0.0105301	Paxs	655.35	Joback Method
dvisc	0.0106601	Paxs	692.15	Joback Method
dvisc	0.0107783	Paxs	728.95	Joback Method
dvisc	0.0108863	Paxs	765.75	Joback Method
dvisc	0.0109853	Paxs	802.55	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C59004716&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
mvol:	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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