11H-Indeno[2,1-a]phenanthrene

Inchi: InChI=1S/C21H14/c1-3-7-16-14(5-1)9-10-20-18(16)11-12-19-17-8-4-2-6-15(17)13-21(19)
InchiKey: JPAMAQWNSMPRLT-UHFFFAOYSA-N
Formula: C21H14
SMILES: c1ccc2c(c1)Cc1c-2ccc2c1ccc1ccccc12
Mol. weight [g/mol]: 266.34
CAS: 220-97-3

Physical Properties

Property code	Value	Unit	Source
gf	618.20	kJ/mol	Joback Method
hf	438.01	kJ/mol	Joback Method
hfus	31.97	kJ/mol	Joback Method
hvap	72.70	kJ/mol	Joback Method
log10ws	-8.03		Crippen Method
logp	5.564		Crippen Method
mcvol	209.450	ml/mol	McGowan Method
pc	2429.05	kPa	Joback Method
rinpol	460.41		NIST Webbook
rinpol	460.41		NIST Webbook
rinpol	460.41		NIST Webbook
tb	793.99	K	Joback Method
tc	1059.55	K	Joback Method
tf	523.97	K	Joback Method
vc	0.814	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	577.34	J/mol×K	793.99	Joback Method
cpg	592.08	J/mol×K	838.25	Joback Method
cpg	606.05	J/mol×K	882.51	Joback Method
cpg	619.52	J/mol×K	926.77	Joback Method
cpg	632.78	J/mol×K	971.03	Joback Method
cpg	646.11	J/mol×K	1015.29	Joback Method

cpg	659.79	J/mol×K	1059.55	Joback Method
dvisc	0.0027321	Pa×s	523.97	Joback Method
dvisc	0.0023996	Pa×s	568.97	Joback Method
dvisc	0.0021481	Pa×s	613.98	Joback Method
dvisc	0.0019522	Pa×s	658.98	Joback Method
dvisc	0.0017960	Pa×s	703.98	Joback Method
dvisc	0.0016690	Pa×s	748.99	Joback Method
dvisc	0.0015639	Pa×s	793.99	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C220973&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

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

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