INDENO[1,2,3-CD]FLUORANTHENE

Inchi: InChI=1S/C22H12/c1-2-6-14-13(5-1)17-9-10-19-15-7-3-4-8-16(15)20-12-11-18(14)21(17)
InchiKey: XAKRHFYJDSMEMI-UHFFFAOYSA-N
Formula: C22H12
SMILES: c1ccc2c(c1)-c1ccc3c4c(ccc-2c14)-c1ccccc1-3
Mol. weight [g/mol]: 276.34

Physical Properties

Property code	Value	Unit	Source
af	0.6560		Cheméo Relay (1.0)
hf	410.61	kJ/mol	Cheméo Relay (1.0)
hfus	36.27	kJ/mol	Joback Method
hvap	128.24	kJ/mol	Cheméo Relay (1.0)
ie	7.60	eV	Cheméo Relay (1.0)
log10ws	-8.73		Cheméo Relay (1.0)
logp	6.135		Crippen Method
mcvol	208.380	ml/mol	McGowan Method
pc	2485.07	kPa	Joback Method
rinpol	484.67		NIST Webbook
rinpol	490.85		NIST Webbook
rinpol	488.38		NIST Webbook
rinpol	488.38		NIST Webbook
tb	775.92	K	Cheméo Relay (1.0)
tc	1099.50	K	Cheméo Relay (1.0)
tf	512.46	K	Cheméo Relay (1.0)
vc	0.859	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	573.06	J/mol×K	828.86	Joback Method
cpg	658.14	J/mol×K	1092.51	Joback Method
cpg	641.76	J/mol×K	1048.57	Joback Method
cpg	626.73	J/mol×K	1004.62	Joback Method
cpg	612.69	J/mol×K	960.68	Joback Method

cpg	599.31	J/mol×K	916.74	Joback Method
cpg	586.21	J/mol×K	872.80	Joback Method
dvisc	0.0082380	Pa×s	709.56	Joback Method
dvisc	0.0081374	Pa×s	828.86	Joback Method
dvisc	0.0081674	Pa×s	789.09	Joback Method
dvisc	0.0082008	Pa×s	749.33	Joback Method
dvisc	0.0083814	Pa×s	590.26	Joback Method
dvisc	0.0082799	Pa×s	669.79	Joback Method
dvisc	0.0083273	Pa×s	630.03	Joback Method
hfust	23.20	kJ/mol	542.30	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C193431&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):

Legend

af: Acentric Factor
cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hfust: Enthalpy of fusion at a given temperature
hvap: Enthalpy of vaporization at standard conditions
ie: Ionization energy
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