Cyclopenta[cd]pyrene

Other names:	Acepyrene
	Acepyrylene
	Cyclopenteno(c,d)pyrene
	4H-Cyclopenta[cd]pyrene
Inchi:	InChI=1S/C18H10/c1-2-11-4-6-13-7-5-12-8-9-15-10-14(3-1)16(11)18(13)17(12)15/h1-10H
InchiKey:	BZCXQYVNASLLQO-UHFFFAOYSA-N
Formula:	C18H10
SMILES:	C1=Cc2cc3cccc4ccc5ccc1c2c5c43
Mol. weight [g/mol]:	226.27
CAS:	27208-37-3

Physical Properties

Property code	Value	Unit	Source
gf	599.28	kJ/mol	Joback Method
hf	460.63	kJ/mol	Joback Method
hfus	29.28	kJ/mol	Joback Method
hvap	65.21	kJ/mol	Joback Method
log10ws	-7.15		Crippen Method
logp	5.068		Crippen Method
mcvol	171.480	ml/mol	McGowan Method
pc	2915.53	kPa	Joback Method
rinpol	396.54		NIST Webbook
rinpol	397.36		NIST Webbook
rinpol	397.93		NIST Webbook
rinpol	398.17		NIST Webbook
rinpol	398.41		NIST Webbook
rinpol	397.57		NIST Webbook
rinpol	395.20		NIST Webbook
rinpol	397.60		NIST Webbook
rinpol	397.15		NIST Webbook
rinpol	396.55		NIST Webbook
rinpol	391.10		NIST Webbook
rinpol	397.04		NIST Webbook
rinpol	391.10		NIST Webbook
rinpol	396.55		NIST Webbook
rinpol	397.04		NIST Webbook
rinpol	397.15		NIST Webbook

rinpol	391.10		NIST Webbook
rinpol	397.90		NIST Webbook
rinpol	397.80		NIST Webbook
rinpol	397.63		NIST Webbook
rinpol	396.68		NIST Webbook
rinpol	397.36		NIST Webbook
rinpol	398.10		NIST Webbook
rinpol	396.54		NIST Webbook
rinpol	397.04		NIST Webbook
tb	713.38	K	Joback Method
tc	970.65	K	Joback Method
tf	499.96	K	Joback Method
vc	0.683	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	438.90	J/mol×K	713.38	Joback Method
cpg	450.85	J/mol×K	756.26	Joback Method
cpg	462.05	J/mol×K	799.14	Joback Method
cpg	472.76	J/mol×K	842.01	Joback Method
cpg	483.28	J/mol×K	884.89	Joback Method
cpg	493.87	J/mol×K	927.77	Joback Method
cpg	504.82	J/mol×K	970.65	Joback Method
dvisc	0.0043451	Pa×s	499.96	Joback Method
dvisc	0.0043262	Pa×s	535.53	Joback Method
dvisc	0.0043098	Pa×s	571.10	Joback Method
dvisc	0.0042953	Pa×s	606.67	Joback Method
dvisc	0.0042825	Pa×s	642.24	Joback Method
dvisc	0.0042710	Pa×s	677.81	Joback Method
dvisc	0.0042607	Pa×s	713.38	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C27208373&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