Pyrene, 4,5-dihydro-

Other names: 4,5-Dihydropyrene
4,5-Ethanophenanthrene
Inchi: InChI=1S/C16H12/c1-3-11-7-9-13-5-2-6-14-10-8-12(4-1)15(11)16(13)14/h1-7,9H,8,10H2
InchiKey: WPCIUCNVWJNRCD-UHFFFAOYSA-N
Formula: C16H12
SMILES: c1cc2c3c(c1)ccc1cccc(c13)CC2
Mol. weight [g/mol]: 204.27
CAS: 6628-98-4

Physical Properties

Property code	Value	Unit	Source
gf	461.22	kJ/mol	Joback Method
hf	309.99	kJ/mol	Joback Method
hfus	23.27	kJ/mol	Joback Method
hvap	58.80	kJ/mol	Joback Method
log10ws	-5.74		Crippen Method
logp	4.092		Crippen Method
mcvol	162.760	ml/mol	McGowan Method
pc	2953.69	kPa	Joback Method
rinpol	330.01		NIST Webbook
rinpol	330.01		NIST Webbook
rinpol	2094.40		NIST Webbook
rinpol	342.18		NIST Webbook
rinpol	327.10		NIST Webbook
rinpol	327.10		NIST Webbook
rinpol	2070.00		NIST Webbook
rinpol	2070.00		NIST Webbook
rinpol	2059.70		NIST Webbook
tb	652.20	K	Joback Method
tc	905.80	K	Joback Method
tf	425.16	K	Joback Method
vc	0.633	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	410.09	J/mol×K	652.20	Joback Method
cpg	424.65	J/mol×K	694.47	Joback Method
cpg	438.02	J/mol×K	736.73	Joback Method
cpg	450.39	J/mol×K	779.00	Joback Method
cpg	461.97	J/mol×K	821.27	Joback Method
cpg	472.96	J/mol×K	863.54	Joback Method
cpg	483.57	J/mol×K	905.80	Joback Method
dvisc	0.0021032	Pa×s	425.16	Joback Method
dvisc	0.0018669	Pa×s	463.00	Joback Method
dvisc	0.0016873	Pa×s	500.84	Joback Method
dvisc	0.0015468	Pa×s	538.68	Joback Method
dvisc	0.0014342	Pa×s	576.52	Joback Method
dvisc	0.0013423	Pa×s	614.36	Joback Method
dvisc	0.0012660	Pa×s	652.20	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C6628984&Units=SI

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