2-ISOPROPYL-10-METHYLPHENANTHRENE

Inchi: InChI=1S/C18H18/c1-12(2)14-8-9-17-16-7-5-4-6-15(16)10-13(3)18(17)11-14/h4-12H,1-3
InchiKey: VNYQWKJAFNCEBZ-UHFFFAOYSA-N
Formula: C18H18
SMILES: Cc1cc2ccccc2c2ccc(C(C)C)cc12
Mol. weight [g/mol]: 234.34

Physical Properties

Property code	Value	Unit	Source
af	0.5388		Cheméo Relay (1.0)
hf	103.86	kJ/mol	Cheméo Relay (1.0)
hfus	25.77	kJ/mol	Joback Method
hvap	95.05	kJ/mol	Cheméo Relay (1.0)
ie	7.61	eV	Cheméo Relay (1.0)
log10ws	-6.85		Cheméo Relay (1.0)
logp	5.425		Crippen Method
mcvol	201.800	ml/mol	McGowan Method
pc	2139.38	kPa	Joback Method
tb	658.02	K	Cheméo Relay (1.0)
tc	905.85	K	Cheméo Relay (1.0)
tf	365.93	K	Cheméo Relay (1.0)
vc	0.755	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	533.01	J/mol×K	690.38	Joback Method
cpg	549.91	J/mol×K	730.26	Joback Method
cpg	565.63	J/mol×K	770.14	Joback Method
cpg	580.29	J/mol×K	810.03	Joback Method
cpg	594.01	J/mol×K	849.91	Joback Method
cpg	606.91	J/mol×K	889.79	Joback Method
cpg	619.11	J/mol×K	929.67	Joback Method
dvisc	0.0013642	Pa×s	407.00	Joback Method
dvisc	0.0009718	Pa×s	454.23	Joback Method

dvisc	0.0007380	Pa×s	501.46	Joback Method
dvisc	0.0005876	Pa×s	548.69	Joback Method
dvisc	0.0004850	Pa×s	595.92	Joback Method
dvisc	0.0004118	Pa×s	643.15	Joback Method
dvisc	0.0003576	Pa×s	690.38	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C66552974&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

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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume