

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:	<chem>Cc1cc2ccccc2c2ccc(C(C)C)cc12</chem>
Mol. weight [g/mol]:	234.34
CAS:	66552-97-4

Physical Properties

Property code	Value	Unit	Source
gf	395.06	kJ/mol	Joback Method
hf	164.13	kJ/mol	Joback Method
hfus	25.77	kJ/mol	Joback Method
hvap	62.82	kJ/mol	Joback Method
log10ws	-6.74		Crippen Method
logp	5.425		Crippen Method
mcvol	201.800	ml/mol	McGowan Method
pc	2139.38	kPa	Joback Method
tb	690.38	K	Joback Method
tc	929.67	K	Joback Method
tf	407.00	K	Joback Method
vc	0.773	m3/kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0007380	Paxs	501.46	Joback Method
dvisc	0.0005876	Paxs	548.69	Joback Method
dvisc	0.0004850	Paxs	595.92	Joback Method
dvisc	0.0004118	Paxs	643.15	Joback Method
dvisc	0.0003576	Paxs	690.38	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C66552974&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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