Retene

Other names:	1-Methyl-7-(1-methylethyl)phenanthrene
	1-Methyl-7-isopropylphenanthrene
	7-Isopropyl-1-methylphenanthrene
	Methyl-1-isopropyl-7-phenanthrene
	NCI-C55390
	NSC 26317
	Phenanthrene, 1-methyl-7-(1-methylethyl)-
	Phenanthrene, 7-isopropyl-1-methyl-
	Reten
	Retene(1-methyl-7-isopropylphenanthrene)
Inchi:	InChI=1S/C18H18/c1-12(2)14-7-10-17-15(11-14)8-9-16-13(3)5-4-6-18(16)17/h4-12H,1-3
InchiKey:	NXLOLUFNDSBYTP-UHFFFAOYSA-N
Formula:	C18H18
SMILES:	Cc1cccc2c1ccc1cc(C(C)C)ccc12
Mol. weight [g/mol]:	234.34
CAS:	483-65-8

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
rinpol	365.96		NIST Webbook
rinpol	368.90		NIST Webbook
rinpol	358.22		NIST Webbook
rinpol	368.67		NIST Webbook
rinpol	368.22		NIST Webbook
rinpol	355.93		NIST Webbook
rinpol	367.31		NIST Webbook
rinpol	368.67		NIST Webbook
rinpol	2176.00		NIST Webbook
tb	663.20	K	NIST Webbook

tc	929.67	K	Joback Method
tf	369.00 ± 0.20	K	NIST Webbook
vc	0.773	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	619.11	J/mol×K	929.67	Joback Method
cpg	606.91	J/mol×K	889.79	Joback Method
cpg	594.01	J/mol×K	849.91	Joback Method
cpg	580.29	J/mol×K	810.03	Joback Method
cpg	565.63	J/mol×K	770.14	Joback Method
cpg	549.91	J/mol×K	730.26	Joback Method
cpg	533.01	J/mol×K	690.38	Joback Method
cps	294.60	J/mol×K	298.10	NIST Webbook
dvisc	0.0004850	Pa×s	595.92	Joback Method
dvisc	0.0005876	Pa×s	548.69	Joback Method
dvisc	0.0003576	Pa×s	690.38	Joback Method
dvisc	0.0009718	Pa×s	454.23	Joback Method
dvisc	0.0013642	Pa×s	407.00	Joback Method
dvisc	0.0004118	Pa×s	643.15	Joback Method
dvisc	0.0007380	Pa×s	501.46	Joback Method
hfust	18.03	kJ/mol	369.00	NIST Webbook
hfust	18.03	kJ/mol	369.00	NIST Webbook
hfust	18.03	kJ/mol	369.00	NIST Webbook
hvapt	54.00	kJ/mol	608.50	NIST Webbook
sfust	48.90	J/mol×K	369.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.38591e+01
Coeff. B	-5.05071e+03
Coeff. C	-1.28244e+02
Temperature range (K), min.	500.15
Temperature range (K), max.	719.15

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C483658&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
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
cps:	Solid phase 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
hfust:	Enthalpy of fusion at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
sfust:	Entropy of fusion at a given temperature
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume