Anthracene, 9-phenyl-

Other names: 9-Phenylanthracene
Inchi: InChI=1S/C20H14/c1-2-8-15(9-3-1)20-18-12-6-4-10-16(18)14-17-11-5-7-13-19(17)20/h1-
InchiKey: LUBXLGUQZVKOFP-UHFFFAOYSA-N
Formula: C20H14
SMILES: c1ccc(-c2c3ccccc3cc3ccccc23)cc1
Mol. weight [g/mol]: 254.33
CAS: 602-55-1

Physical Properties

Property code	Value	Unit	Source
gf	536.38	kJ/mol	Joback Method
hf	376.13	kJ/mol	Joback Method
hfus	28.90	kJ/mol	Joback Method
hvap	69.27	kJ/mol	Joback Method
ie	7.25	eV	NIST Webbook
ie	7.25	eV	NIST Webbook
log10ws	-7.68		Crippen Method
logp	5.660		Crippen Method
mcvol	206.220	ml/mol	McGowan Method
pc	2460.47	kPa	Joback Method
rinpol	396.38		NIST Webbook
rinpol	396.05		NIST Webbook
rinpol	406.90		NIST Webbook
rinpol	406.47		NIST Webbook
rinpol	406.47		NIST Webbook
rinpol	396.38		NIST Webbook
rinpol	394.37		NIST Webbook
rinpol	395.50		NIST Webbook
rinpol	394.37		NIST Webbook
rinpol	2374.00		NIST Webbook
tb	690.20	K	NIST Webbook
tc	1028.40	K	Joback Method
tf	423.00 ± 3.00	K	NIST Webbook
tf	425.00 ± 3.00	K	NIST Webbook
tf	427.60 ± 0.80	K	NIST Webbook
vc	0.783	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	552.94	J/mol×K	758.28	Joback Method
cpg	622.13	J/mol×K	983.38	Joback Method
cpg	610.08	J/mol×K	938.36	Joback Method
cpg	597.34	J/mol×K	893.34	Joback Method
cpg	583.72	J/mol×K	848.32	Joback Method
cpg	568.99	J/mol×K	803.30	Joback Method
cpg	633.72	J/mol×K	1028.40	Joback Method
dvisc	0.0009631	Pa×s	508.41	Joback Method
dvisc	0.0007314	Pa×s	558.39	Joback Method
dvisc	0.0005812	Pa×s	608.36	Joback Method
dvisc	0.0004782	Pa×s	658.33	Joback Method
dvisc	0.0004045	Pa×s	708.31	Joback Method
dvisc	0.0013464	Pa×s	458.44	Joback Method
dvisc	0.0003497	Pa×s	758.28	Joback Method
hsubt	115.30	kJ/mol	389.50	NIST Webbook
hsubt	119.70	kJ/mol	373.50	NIST Webbook
hsubt	118.70	kJ/mol	383.00	NIST Webbook
hvapt	84.40	kJ/mol	470.00	NIST Webbook
hvapt	86.20	kJ/mol	474.00	NIST Webbook
hvapt	91.60	kJ/mol	398.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	2.57575e+01
Coeff. B	-1.07072e+04
Coeff. C	-9.91840e+01
Temperature range (K), min.	519.57
Temperature range (K), max.	622.86

Sources

Solubilities of Triptycene, 9-Phenylanthracene, 9,10-Dimethylanthracene, and 2-Methylanthracene in Pressurized Hot Water at Temperatures from 313 K to the Melting Point:	https://www.doi.org/10.1021/je700447m
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=C602551&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

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
hsubt:	Enthalpy of sublimation at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume