5,6,11,12-Tetraphenylnaphthacene

Other names:	5,6,11,12-Tetraphenyltetracene
	Naphthacene, 5,6,11,12-tetraphenyl-
	Rubren
	Rubrene
Inchi:	InChI=1S/C42H28/c1-5-17-29(18-6-1)37-33-25-13-14-26-34(33)39(31-21-9-3-10-22-31)4
InchiKey:	YYMBJDOZVAITBP-UHFFFAOYSA-N
Formula:	C42H28
SMILES:	c1ccc(-c2c3ccccc3c(-c3ccccc3)c3c(-c4ccccc4)c4ccccc4c(-c4ccccc4)c23)cc1
Mol. weight [g/mol]:	532.67
CAS:	517-51-1

Physical Properties

Property code	Value	Unit	Source
chs	-21149.00 ± 21.00	kJ/mol	NIST Webbook
gf	1126.98	kJ/mol	Joback Method
hf	882.00	kJ/mol	NIST Webbook
hfs	620.00 ± 22.00	kJ/mol	NIST Webbook
hfs	620.00 ± 21.00	kJ/mol	NIST Webbook
hfus	63.46	kJ/mol	Joback Method
hsub	262.00	kJ/mol	NIST Webbook
hvap	129.36	kJ/mol	Joback Method
ie	6.41	eV	NIST Webbook
log10ws	-17.30		Crippen Method
logp	11.814		Crippen Method
mcvol	425.460	ml/mol	McGowan Method
pc	1149.10	kPa	Joback Method
tb	1380.58	K	Joback Method
tc	1695.98	K	Joback Method
tf	868.42	K	Joback Method
vc	1.613	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	1698.97	J/mol×K	1643.42	Joback Method
cpg	1648.56	J/mol×K	1590.85	Joback Method
cpg	1603.47	J/mol×K	1538.28	Joback Method
cpg	1563.09	J/mol×K	1485.71	Joback Method
cpg	1526.79	J/mol×K	1433.15	Joback Method
cpg	1493.96	J/mol×K	1380.58	Joback Method
cpg	1755.33	J/mol×K	1695.98	Joback Method
dvisc	0.0003065	Pa×s	868.42	Joback Method
dvisc	0.0000771	Pa×s	1380.58	Joback Method
dvisc	0.0000899	Pa×s	1295.22	Joback Method
dvisc	0.0001072	Pa×s	1209.86	Joback Method
dvisc	0.0001313	Pa×s	1124.50	Joback Method
dvisc	0.0001663	Pa×s	1039.14	Joback Method
dvisc	0.0002197	Pa×s	953.78	Joback Method
hsubt	160.60 ± 4.20	kJ/mol	488.00	NIST Webbook
hsubt	162.80 ± 4.20	kJ/mol	453.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	2.26410e+01
Coeff. B	-1.47679e+04
Temperature range (K), min.	660.66
Temperature range (K), max.	852.18

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C517511&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

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
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
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume