Dibenzo[g,p]chrysene

Other names: 1,2,3,4,5,6,7,8-Tetrabenzonaphthalene
Dibenzo(a,c)triphenylene
Tetrabenzonaphthalene
Inchi: InChI=1S/C26H16/c1-5-13-21-17(9-1)18-10-2-6-14-22(18)26-24-16-8-4-12-20(24)19-11-3
InchiKey: GQDKQZAEQBGVBS-UHFFFAOYSA-N
Formula: C26H16
SMILES: c1ccc2c(c1)c1ccccc1c1c3ccccc3c3ccccc3c21
Mol. weight [g/mol]: 328.41
CAS: 191-68-4

Physical Properties

Property code	Value	Unit	Source
chs	-12897.00	kJ/mol	NIST Webbook
gf	775.18	kJ/mol	Joback Method
hf	503.00	kJ/mol	NIST Webbook
hfs	379.00 ± 37.00	kJ/mol	NIST Webbook
hfus	40.68	kJ/mol	Joback Method
hsub	150.90	kJ/mol	NIST Webbook
hsub	195.00	kJ/mol	NIST Webbook
hvap	86.59	kJ/mol	Joback Method
ie	7.42	eV	NIST Webbook
ie	7.26	eV	NIST Webbook
ie	7.18 ± 0.04	eV	NIST Webbook
ie	7.58	eV	NIST Webbook
ie	7.20	eV	NIST Webbook
ie	7.20 ± 0.02	eV	NIST Webbook
log10ws	-10.49		Crippen Method
logp	7.453		Crippen Method
mcvol	256.140	ml/mol	McGowan Method
pc	2032.72	kPa	Joback Method
rinpol	566.87		NIST Webbook
rinpol	567.47		NIST Webbook
tb	935.78	K	Joback Method
tc	1209.93	K	Joback Method
tf	491.00 ± 4.00	K	NIST Webbook
vc	0.994	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	753.48	J/mol×K	935.78	Joback Method
cpg	769.57	J/mol×K	981.47	Joback Method
cpg	785.72	J/mol×K	1027.16	Joback Method
cpg	802.30	J/mol×K	1072.85	Joback Method
cpg	819.68	J/mol×K	1118.55	Joback Method
cpg	838.20	J/mol×K	1164.24	Joback Method
cpg	858.23	J/mol×K	1209.93	Joback Method
dvisc	0.0027637	Pa×s	674.95	Joback Method
dvisc	0.0031676	Pa×s	622.78	Joback Method
dvisc	0.0024589	Pa×s	727.11	Joback Method
dvisc	0.0022223	Pa×s	779.28	Joback Method
dvisc	0.0020341	Pa×s	831.45	Joback Method
dvisc	0.0018814	Pa×s	883.61	Joback Method
dvisc	0.0017553	Pa×s	935.78	Joback Method
hsubt	142.20	kJ/mol	450.50	NIST Webbook
hsubt	141.80	kJ/mol	458.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	4.28931e+01
Coeff. B	-2.55909e+04
Coeff. C	-5.68200e+00
Temperature range (K), min.	606.33
Temperature range (K), max.	686.63

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C191684&Units=SI

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume