Dibenzo(h,rst)pentaphene

Other names:	Tribenzo(a,e,i)pyrene
	(1,2:4,5:7,8)-Tribenzopyrene
Inchi:	InChI=1S/C28H16/c1-3-9-19-17(7-1)15-25-21-11-5-6-12-22(21)26-16-18-8-2-4-10-20(18)
InchiKey:	LMNAZSSKDBUVFA-UHFFFAOYSA-N
Formula:	C28H16
SMILES:	c1ccc2c(c1)cc1c3ccccc3c3cc4ccccc4c4ccc2c1c43
Mol. weight [g/mol]:	352.43
CAS:	192-47-2

Physical Properties

Property code	Value	Unit	Source
gf	883.28	kJ/mol	Joback Method
hf	658.89	kJ/mol	Joback Method
hfus	45.46	kJ/mol	Joback Method
hvap	92.71	kJ/mol	Joback Method
ie	6.99	eV	NIST Webbook
ie	7.38	eV	NIST Webbook
ie	7.17	eV	NIST Webbook
log10ws	-11.71		Crippen Method
logp	8.044		Crippen Method
mcvol	269.160	ml/mol	McGowan Method
pc	1947.51	kPa	Joback Method
tb	997.80	K	Joback Method
tc	1271.87	K	Joback Method
tf	608.00 ± 1.00	K	NIST Webbook
vc	1.058	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	812.33	J/mol×K	997.80	Joback Method
cpg	830.69	J/mol×K	1043.48	Joback Method
cpg	850.20	J/mol×K	1089.16	Joback Method
cpg	871.30	J/mol×K	1134.83	Joback Method

cpg	894.41	J/mol×K	1180.51	Joback Method
cpg	919.98	J/mol×K	1226.19	Joback Method
cpg	948.44	J/mol×K	1271.87	Joback Method
dvisc	0.0086256	Pa×s	696.82	Joback Method
dvisc	0.0081349	Pa×s	746.98	Joback Method
dvisc	0.0077289	Pa×s	797.15	Joback Method
dvisc	0.0073878	Pa×s	847.31	Joback Method
dvisc	0.0070975	Pa×s	897.47	Joback Method
dvisc	0.0068476	Pa×s	947.64	Joback Method
dvisc	0.0066304	Pa×s	997.80	Joback Method
hfust	28.80	kJ/mol	608.00	NIST Webbook

Sources

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=C192472&Units=SI
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
hfust: Enthalpy of fusion 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
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume