Dibenzo(a,i)pyrene

Other names:	3,4:9,10-Dibenzopyrene
	Benzo[rst]pentaphene
	DB(a,i)P
	Dibenzo-3,4,9,10-pyrene
	Dibenz(a,i)pyrene
	1,2,7,8-Dibenzopyrene
	3,4,9,10-Dibenzopyrene
	3,4:9,10-Dibenzpyrene
	Dibenzo(b,h)pyrene
	1,2:7,8-Dibenzpyrene
	Rcra waste number U064
	3,4,9,10-Dibenzpyrene
	NSC 87521
Inchi:	InChI=1S/C24H14/c1-3-7-19-15(5-1)13-17-9-10-18-14-16-6-2-4-8-20(16)22-12-11-21(19)
InchiKey:	TUGYIJVAYAHHHM-UHFFFAOYSA-N
Formula:	C24H14
SMILES:	c1ccc2c(c1)cc1ccc3cc4ccccc4c4ccc2c1c34
Mol. weight [g/mol]:	302.37
CAS:	189-55-9

Physical Properties

Property code	Value	Unit	Source
gf	752.58	kJ/mol	Joback Method
hf	561.85	kJ/mol	Joback Method
hfus	38.47	kJ/mol	Joback Method
hvap	81.51	kJ/mol	Joback Method
ie	7.30	eV	NIST Webbook
ie	7.06	eV	NIST Webbook
ie	6.95	eV	NIST Webbook
ie	7.07 ± 0.04	eV	NIST Webbook
log10ws	-9.91		Crippen Method
logp	6.890		Crippen Method
mcvol	232.260	ml/mol	McGowan Method
pc	2241.88	kPa	Joback Method
rinpol	558.11		NIST Webbook
rinpol	3526.00		NIST Webbook
rinpol	3570.00		NIST Webbook

rinpol	3570.00		NIST Webbook
rinpol	556.47		NIST Webbook
rinpol	557.20		NIST Webbook
rinpol	560.34		NIST Webbook
rinpol	556.32		NIST Webbook
rinpol	556.32		NIST Webbook
rinpol	556.47		NIST Webbook
rinpol	586.40		NIST Webbook
rinpol	556.47		NIST Webbook
rinpol	3526.00		NIST Webbook
rinpol	3526.00		NIST Webbook
tb	882.32	K	Joback Method
tc	1151.38	K	Joback Method
tf	556.80 ± 0.10	K	NIST Webbook
vc	0.911	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	739.36	J/mol×K	1106.54	Joback Method
cpg	757.84	J/mol×K	1151.38	Joback Method
cpg	661.66	J/mol×K	882.32	Joback Method
cpg	676.44	J/mol×K	927.16	Joback Method
cpg	691.24	J/mol×K	972.01	Joback Method
cpg	706.42	J/mol×K	1016.85	Joback Method
cpg	722.35	J/mol×K	1061.69	Joback Method
dvisc	0.0039222	Pa×s	882.32	Joback Method
dvisc	0.0040664	Pa×s	836.35	Joback Method
dvisc	0.0052883	Pa×s	606.52	Joback Method
dvisc	0.0049439	Pa×s	652.49	Joback Method
dvisc	0.0046630	Pa×s	698.45	Joback Method
dvisc	0.0044300	Pa×s	744.42	Joback Method
dvisc	0.0042338	Pa×s	790.39	Joback Method
hfust	27.87	kJ/mol	556.80	NIST Webbook
hfust	27.87	kJ/mol	556.80	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	548.00	K	0.01	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C189559&Units=SI
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

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