Dibenzo[def,mno]chrysene

Other names:	Anthanthrene
	Anthanthren
	Dibenzo[cd,jk]pyrene
	Anthranthrene
	Dibenz[def,mno]chrysene
	Dibenzo[def,mmo]chrysene
Inchi:	InChI=1S/C22H12/c1-3-13-7-9-18-12-16-6-2-4-14-8-10-17-11-15(5-1)19(13)21(18)22(17)
InchiKey:	YFIJJNAKSZUOLT-UHFFFAOYSA-N
Formula:	C22H12
SMILES:	c1cc2ccc3cc4cccc5ccc6cc(c1)c2c3c6c54
Mol. weight [g/mol]:	276.33
CAS:	191-26-4

Physical Properties

Property code	Value	Unit	Source
gf	729.98	kJ/mol	Joback Method
hf	557.67	kJ/mol	Joback Method
hfus	36.27	kJ/mol	Joback Method
hvap	76.42	kJ/mol	Joback Method
ie	7.01	eV	NIST Webbook
ie	6.84	eV	NIST Webbook
ie	6.92 ± 0.04	eV	NIST Webbook
ie	7.10	eV	NIST Webbook
ie	7.11	eV	NIST Webbook
log10ws	-9.32		Crippen Method
logp	6.328		Crippen Method
mcvol	208.380	ml/mol	McGowan Method
pc	2485.07	kPa	Joback Method
rinpol	504.85		NIST Webbook
rinpol	503.90		NIST Webbook
rinpol	509.50		NIST Webbook
rinpol	3215.00		NIST Webbook
rinpol	3215.00		NIST Webbook
rinpol	3183.00		NIST Webbook
rinpol	3186.00		NIST Webbook
rinpol	3215.00		NIST Webbook
rinpol	503.89		NIST Webbook

rinpol	508.40		NIST Webbook
rinpol	505.29		NIST Webbook
rinpol	3215.00		NIST Webbook
rinpol	504.26		NIST Webbook
rinpol	505.29		NIST Webbook
rinpol	504.10		NIST Webbook
rinpol	503.89		NIST Webbook
rinpol	505.97		NIST Webbook
rinpol	505.29		NIST Webbook
rinpol	505.97		NIST Webbook
rinpol	506.40		NIST Webbook
rinpol	505.61		NIST Webbook
rinpol	503.90		NIST Webbook
rinpol	505.97		NIST Webbook
rinpol	508.40		NIST Webbook
rinpol	505.49		NIST Webbook
rinpol	506.49		NIST Webbook
rinpol	509.50		NIST Webbook
rinpol	510.00		NIST Webbook
rinpol	510.58		NIST Webbook
rinpol	503.89		NIST Webbook
rinpol	508.40		NIST Webbook
tb	828.86	K	Joback Method
tc	1092.51	K	Joback Method
tf	530.90 ± 1.50	K	NIST Webbook
vc	0.830	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	658.14	J/mol×K	1092.51	Joback Method
cpg	573.06	J/mol×K	828.86	Joback Method
cpg	586.21	J/mol×K	872.80	Joback Method
cpg	599.31	J/mol×K	916.74	Joback Method
cpg	612.69	J/mol×K	960.68	Joback Method
cpg	626.73	J/mol×K	1004.62	Joback Method
cpg	641.76	J/mol×K	1048.57	Joback Method
dvisc	0.0081374	Pa×s	828.86	Joback Method
dvisc	0.0083814	Pa×s	590.26	Joback Method
dvisc	0.0083273	Pa×s	630.03	Joback Method
dvisc	0.0082799	Pa×s	669.79	Joback Method

dvisc	0.0082380	Pa×s	709.56	Joback Method
dvisc	0.0082008	Pa×s	749.33	Joback Method
dvisc	0.0081674	Pa×s	789.09	Joback Method
hsubt	135.00 ± 5.00	kJ/mol	479.00	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C191264&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
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume