PENTAPHENE

Other names: pentapheno
Inchi: InChI=1S/C22H14/c1-3-7-17-13-21-19(11-15(17)5-1)9-10-20-12-16-6-2-4-8-18(16)14-22(
InchiKey: JQQSUOJIMKJQHS-UHFFFAOYSA-N
Formula: C22H14
SMILES: c1ccc2cc3c(ccc4cc5ccccc5cc43)cc2c1
Mol. weight [g/mol]: 278.35

Physical Properties

Property code	Value	Unit	Source
af	0.6067		Cheméo Relay (1.0)
gf	644.48	kJ/mol	Joback Method
hf	361.10	kJ/mol	Cheméo Relay (1.0)
hfus	33.69	kJ/mol	Joback Method
hvap	131.18	kJ/mol	Cheméo Relay (1.0)
ie	7.35	eV	NIST Webbook
ie	7.27	eV	NIST Webbook
ie	7.27	eV	NIST Webbook
ie	7.27 ± 0.02	eV	NIST Webbook
ie	7.53	eV	NIST Webbook
ie	7.34 ± 0.04	eV	NIST Webbook
log10ws	-9.02		Cheméo Relay (1.0)
logp	6.299		Crippen Method
mcvol	219.240	ml/mol	McGowan Method
pc	2347.36	kPa	Joback Method
rinpol	496.67		NIST Webbook
rinpol	496.83		NIST Webbook
rinpol	496.67		NIST Webbook
rinpol	496.83		NIST Webbook
rinpol	495.80		NIST Webbook
rinpol	496.67		NIST Webbook
rinpol	496.83		NIST Webbook
rinpol	496.83		NIST Webbook
tb	796.59	K	Cheméo Relay (1.0)
tc	1100.27	K	Cheméo Relay (1.0)
tf	563.58	K	Cheméo Relay (1.0)
vc	0.836	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	607.64	J/mol×K	820.30	Joback Method
cpg	622.45	J/mol×K	865.23	Joback Method
cpg	636.52	J/mol×K	910.16	Joback Method
cpg	650.13	J/mol×K	955.09	Joback Method
cpg	663.56	J/mol×K	1000.03	Joback Method
cpg	677.10	J/mol×K	1044.96	Joback Method
cpg	691.04	J/mol×K	1089.89	Joback Method
dvisc	0.0022584	Pa×s	532.48	Joback Method
dvisc	0.0019125	Pa×s	580.45	Joback Method
dvisc	0.0016611	Pa×s	628.42	Joback Method
dvisc	0.0014719	Pa×s	676.39	Joback Method
dvisc	0.0013254	Pa×s	724.36	Joback Method
dvisc	0.0012090	Pa×s	772.33	Joback Method
dvisc	0.0011148	Pa×s	820.30	Joback Method

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C222935&Units=SI

Legend

af: Acentric Factor
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
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