Benzo[h]pentaphene

Inchi: InChI=1S/C26H16/c1-3-9-19-15-25-23(13-17(19)7-1)21-11-5-6-12-22(21)24-14-18-8-2-4-
InchiKey: FUDUPLHPBBXJRW-UHFFFAOYSA-N
Formula: C26H16
SMILES: c1ccc2cc3c(cc2c1)c1ccccc1c1cc2ccccc2cc13
Mol. weight [g/mol]: 328.41
CAS: 214-91-5

Physical Properties

Property code	Value	Unit	Source
gf	775.18	kJ/mol	Joback Method
hf	566.03	kJ/mol	Joback Method
hfus	40.68	kJ/mol	Joback Method
hvap	86.59	kJ/mol	Joback Method
ie	7.30 ± 0.04	eV	NIST Webbook
ie	7.36 ± 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	590.43		NIST Webbook
rinpol	591.00		NIST Webbook
tb	935.78	K	Joback Method
tc	1209.93	K	Joback Method
tf	622.78	K	Joback Method
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	0.0031676	Pa×s	622.78	Joback Method
dvisc	0.0027637	Pa×s	674.95	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

Sources

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=C214915&Units=SI

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
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

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