Pyranthrene

Inchi: InChI=1S/C30H16/c1-3-7-23-17(5-1)13-19-9-11-22-16-26-24-8-4-2-6-18(24)14-20-10-12-
InchiKey: LNKHTYQPVMAJSF-UHFFFAOYSA-N
Formula: C30H16
SMILES: c1ccc2c(c1)cc1ccc3cc4c5ccccc5cc5ccc6cc2c1c3c6c54
Mol. weight [g/mol]: 376.45
CAS: 191-13-9

Physical Properties

Property code	Value	Unit	Source
gf	991.38	kJ/mol	Joback Method
hf	751.75	kJ/mol	Joback Method
hfus	50.25	kJ/mol	Joback Method
hvap	98.83	kJ/mol	Joback Method
ie	6.98	eV	NIST Webbook
ie	6.99	eV	NIST Webbook
ie	6.69	eV	NIST Webbook
log10ws	-12.93		Crippen Method
logp	8.635		Crippen Method
mcvol	282.180	ml/mol	McGowan Method
pc	1867.55	kPa	Joback Method
tb	1059.82	K	Joback Method
tc	1334.83	K	Joback Method
tf	770.86	K	Joback Method
vc	1.121	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	877.53	J/mol×K	1059.82	Joback Method
cpg	900.56	J/mol×K	1105.65	Joback Method
cpg	926.04	J/mol×K	1151.49	Joback Method
cpg	954.48	J/mol×K	1197.32	Joback Method
cpg	986.42	J/mol×K	1243.16	Joback Method
cpg	1022.37	J/mol×K	1288.99	Joback Method

cpg	1062.84	J/mol×K	1334.83	Joback Method
dvisc	0.0277526	Pa×s	770.86	Joback Method
dvisc	0.0275076	Pa×s	819.02	Joback Method
dvisc	0.0272917	Pa×s	867.18	Joback Method
dvisc	0.0270999	Pa×s	915.34	Joback Method
dvisc	0.0269285	Pa×s	963.50	Joback Method
dvisc	0.0267743	Pa×s	1011.66	Joback Method
dvisc	0.0266349	Pa×s	1059.82	Joback Method
hsubt	194.50 ± 6.70	kJ/mol	595.00	NIST Webbook

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=C191139&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
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
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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