7-Methyldibenzo(a,h)pyrene

Inchi: InChI=1S/C25H16/c1-15-18-7-4-5-9-21(18)23-11-10-17-14-16-6-2-3-8-20(16)22-13-12-19
InchiKey: AIGLSXACYSPHLX-UHFFFAOYSA-N
Formula: C25H16
SMILES: Cc1c2ccccc2c2ccc3cc4ccccc4c4ccc1c2c34
Mol. weight [g/mol]: 316.39
CAS: 5174-22-1

Physical Properties

Property code	Value	Unit	Source
gf	751.37	kJ/mol	Joback Method
hf	529.74	kJ/mol	Joback Method
hfus	40.67	kJ/mol	Joback Method
hvap	84.39	kJ/mol	Joback Method
log10ws	-10.38		Crippen Method
logp	7.199		Crippen Method
mcvol	246.350	ml/mol	McGowan Method
pc	2023.58	kPa	Joback Method
tb	910.18	K	Joback Method
tc	1174.45	K	Joback Method
tf	630.31	K	Joback Method
vc	0.968	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	717.24	J/mol×K	910.18	Joback Method
cpg	732.84	J/mol×K	954.22	Joback Method
cpg	748.57	J/mol×K	998.27	Joback Method
cpg	764.77	J/mol×K	1042.31	Joback Method
cpg	781.78	J/mol×K	1086.36	Joback Method
cpg	799.91	J/mol×K	1130.40	Joback Method
cpg	819.51	J/mol×K	1174.45	Joback Method
dvisc	0.0051440	Pa×s	630.31	Joback Method
dvisc	0.0048054	Pa×s	676.96	Joback Method

dvisc	0.0045287	Pa×s	723.60	Joback Method
dvisc	0.0042987	Pa×s	770.25	Joback Method
dvisc	0.0041048	Pa×s	816.89	Joback Method
dvisc	0.0039392	Pa×s	863.54	Joback Method
dvisc	0.0037962	Pa×s	910.18	Joback Method

Sources

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=C5174221&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
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