

7,14-Dimethyldibenzo(a,h)pyrene

Inchi:	InChI=1S/C26H18/c1-15-17-7-3-5-9-21(17)23-14-12-20-16(2)18-8-4-6-10-22(18)24-13-1
InchiKey:	IMTXKGSVVYLNH-UHFFFAOYSA-N
Formula:	C26H18
SMILES:	<chem>Cc1c2ccccc2c2ccc3c(C)c4ccccc4c4ccc1c2c34</chem>
Mol. weight [g/mol]:	330.42
CAS:	83439-54-7

Physical Properties

Property code	Value	Unit	Source
gf	750.16	kJ/mol	Joback Method
hf	497.63	kJ/mol	Joback Method
hfus	42.88	kJ/mol	Joback Method
hvap	87.28	kJ/mol	Joback Method
log10ws	-10.86		Crippen Method
logp	7.507		Crippen Method
mvol	260.440	ml/mol	McGowan Method
pc	1835.69	kPa	Joback Method
tb	938.04	K	Joback Method
tc	1198.25	K	Joback Method
tf	654.10	K	Joback Method
vc	1.024	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	774.21	J/molxK	938.04	Joback Method
cpg	790.65	J/molxK	981.41	Joback Method
cpg	807.32	J/molxK	1024.78	Joback Method
cpg	824.54	J/molxK	1068.15	Joback Method
cpg	842.61	J/molxK	1111.52	Joback Method
cpg	861.85	J/molxK	1154.88	Joback Method
cpg	882.56	J/molxK	1198.25	Joback Method
dvisc	0.0049821	Paxs	654.10	Joback Method
dvisc	0.0046515	Paxs	701.42	Joback Method

dvisc	0.0043807	Paxs	748.75	Joback Method
dvisc	0.0041552	Paxs	796.07	Joback Method
dvisc	0.0039647	Paxs	843.39	Joback Method
dvisc	0.0038019	Paxs	890.72	Joback Method
dvisc	0.0036612	Paxs	938.04	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=C83439547&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
mccvol:	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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