

5H-Benzo[b]cyclopenta[def]chrysene

Inchi:	InChI=1S/C23H14/c1-3-7-18-15(6-1)12-17-13-21-19-8-4-2-5-14(19)11-16-9-10-20(18)23
InchiKey:	DXPZXOZITNZSNG-UHFFFAOYSA-N
Formula:	C23H14
SMILES:	<chem>c1ccc2c3c4c(ccc5c6ccccc6cc(c54)C3)cc2c1</chem>
Mol. weight [g/mol]:	290.36
CAS:	87308-54-1

Physical Properties

Property code	Value	Unit	Source
gf	726.30	kJ/mol	Joback Method
hf	530.87	kJ/mol	Joback Method
hfus	36.76	kJ/mol	Joback Method
hvap	78.82	kJ/mol	Joback Method
log10ws	-9.04		Crippen Method
logp	6.204		Crippen Method
mcvol	222.470	ml/mol	McGowan Method
pc	2318.07	kPa	Joback Method
tb	856.01	K	Joback Method
tc	1121.31	K	Joback Method
tf	598.01	K	Joback Method
vc	0.877	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	631.13	J/molxK	856.01	Joback Method
cpg	706.40	J/molxK	1077.10	Joback Method
cpg	690.07	J/molxK	1032.88	Joback Method
cpg	674.72	J/molxK	988.66	Joback Method
cpg	660.02	J/molxK	944.44	Joback Method
cpg	645.60	J/molxK	900.23	Joback Method
cpg	724.08	J/molxK	1121.31	Joback Method
dvisc	0.0055010	Paxs	856.01	Joback Method
dvisc	0.0056275	Paxs	813.01	Joback Method

dvisc	0.0057716	Paxs	770.01	Joback Method
dvisc	0.0059371	Paxs	727.01	Joback Method
dvisc	0.0061292	Paxs	684.01	Joback Method
dvisc	0.0063545	Paxs	641.01	Joback Method
dvisc	0.0066224	Paxs	598.01	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C87308541&Units=SI
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

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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