

4H-Benzo[def]cyclopenta[mno]chrysene

Inchi:	InChI=1S/C21H12/c1-3-12-7-8-16-9-13-5-2-6-15-11-17-10-14(4-1)18(12)20(16)21(17)19
InchiKey:	WEKAXSAVALUHAU-UHFFFAOYSA-N
Formula:	C21H12
SMILES:	<chem>c1cc2c3c(c1)cc1ccc4cccc5cc(c3c1c45)C2</chem>
Mol. weight [g/mol]:	264.32
CAS:	59004-72-7

Physical Properties

Property code	Value	Unit	Source
gf	703.70	kJ/mol	Joback Method
hf	526.69	kJ/mol	Joback Method
hfus	34.56	kJ/mol	Joback Method
hvap	73.73	kJ/mol	Joback Method
log10ws	-8.45		Crippen Method
logp	5.641		Crippen Method
mcvol	198.590	ml/mol	McGowan Method
pc	2574.11	kPa	Joback Method
tb	802.55	K	Joback Method
tc	1062.21	K	Joback Method
tf	581.75	K	Joback Method
vc	0.795	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	543.75	J/molxK	802.55	Joback Method
cpg	556.52	J/molxK	845.83	Joback Method
cpg	569.14	J/molxK	889.10	Joback Method
cpg	581.94	J/molxK	932.38	Joback Method
cpg	595.27	J/molxK	975.65	Joback Method
cpg	609.49	J/molxK	1018.93	Joback Method
cpg	624.92	J/molxK	1062.21	Joback Method
dvisc	0.0102272	Paxs	581.75	Joback Method
dvisc	0.0103866	Paxs	618.55	Joback Method

dvisc	0.0105301	Paxs	655.35	Joback Method
dvisc	0.0106601	Paxs	692.15	Joback Method
dvisc	0.0107783	Paxs	728.95	Joback Method
dvisc	0.0108863	Paxs	765.75	Joback Method
dvisc	0.0109853	Paxs	802.55	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=C59004727&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
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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