

Cyclopenta(def)phenanthrenone

Other names:	4H-cyclopenta[def]phenanthren-4-one 4H-cyclopenta[def]phenanthren-4-one
Inchi:	InChI=1S/C15H8O/c16-15-11-5-1-3-9-7-8-10-4-2-6-12(15)14(10)13(9)11/h1-8H
InchiKey:	IFCBMPOMNSORDG-UHFFFAOYSA-N
Formula:	C15H18O
SMILES:	O=c1c2cccc3ccc4cccc1c4c32
Mol. weight [g/mol]:	214.30
CAS:	5737-13-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.14		Crippen Method
logp	3.382		Crippen Method
mcvol	150.240	ml/mol	McGowan Method
rinpol	1977.00		NIST Webbook
rinpol	342.90		NIST Webbook
rinpol	341.20		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	16.30	kJ/mol	443.90	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5737133&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

hfust:	Enthalpy of fusion at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices

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