

# Perylene-D12

<b>Other names:</b>	D12-Perylene (ISTD) Perylene - d Perylene, perdeutero- [2H12]Perylene
<b>Inchi:</b>	InChI=1S/C20H12/c1-5-13-6-2-11-17-18-12-4-8-14-7-3-10-16(20(14)18)15(9-1)19(13)17
<b>InchiKey:</b>	CSHWQDPOILHKBI-AQZSQYOVSA-N
<b>Formula:</b>	C20D12
<b>SMILES:</b>	c1cc2cccc3c4cccc5cccc(c(c1)c23)c54
<b>Mol. weight [g/mol]:</b>	264.38
<b>CAS:</b>	1520-96-3

## Physical Properties

Property code	Value	Unit	Source
gf	621.88	kJ/mol	Joback Method
hf	464.81	kJ/mol	Joback Method
hfus	31.48	kJ/mol	Joback Method
hvap	119.50	kJ/mol	NIST Webbook
log10ws	-8.10		Crippen Method
logp	5.737		Crippen Method
mcvol	195.360	ml/mol	McGowan Method
pc	2608.40	kPa	Joback Method
rinpol	442.30		NIST Webbook
rinpol	456.04		NIST Webbook
rinpol	456.04		NIST Webbook
rinpol	442.30		NIST Webbook
tb	766.84	K	Joback Method
tc	1030.60	K	Joback Method
tf	516.22	K	Joback Method
vc	0.765	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	521.16	J/molxK	766.84	Joback Method

cpg	534.69	J/molxK	810.80	Joback Method
cpg	547.49	J/molxK	854.76	Joback Method
cpg	559.83	J/molxK	898.72	Joback Method
cpg	572.01	J/molxK	942.68	Joback Method
cpg	584.31	J/molxK	986.64	Joback Method
cpg	597.00	J/molxK	1030.60	Joback Method
dvisc	0.0032474	Paxs	516.22	Joback Method
dvisc	0.0029976	Paxs	557.99	Joback Method
dvisc	0.0027980	Paxs	599.76	Joback Method
dvisc	0.0026352	Paxs	641.53	Joback Method
dvisc	0.0025002	Paxs	683.30	Joback Method
dvisc	0.0023865	Paxs	725.07	Joback Method
dvisc	0.0022895	Paxs	766.84	Joback Method
hvapt	119.51	kJ/mol	298.00	Enthalpies of Vaporization and Vapor Pressures of Some Deuterated Hydrocarbons. Liquid-Vapor Pressure Isotope Effects

## Sources

<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>Enthalpies of Vaporization and Vapor Pressures of Some Deuterated Hydrocarbons. Liquid-Vapor Pressure Isotope Effects:</b>	<a href="https://www.doi.org/10.1021/je800091s">https://www.doi.org/10.1021/je800091s</a>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C1520963&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C1520963&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>

## Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>dvisc:</b>	Dynamic viscosity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>hvapt:</b>	Enthalpy of vaporization at a given temperature

<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpol:</b>	Non-polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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