

# Pyrene, 1-decyl-

<b>Other names:</b>	3-n-Decylpyrene 1-decylpyrene
<b>Inchi:</b>	InChI=1S/C26H30/c1-2-3-4-5-6-7-8-9-11-20-14-15-23-17-16-21-12-10-13-22-18-19-24(2
<b>InchiKey:</b>	KIDRHZDFZVQIJA-UHFFFAOYSA-N
<b>Formula:</b>	C26H30
<b>SMILES:</b>	CCCCCCCCCc1ccc2ccc3cccc4ccc1c2c34
<b>Mol. weight [g/mol]:</b>	342.52
<b>CAS:</b>	55682-90-1

## Physical Properties

Property code	Value	Unit	Source
gf	565.75	kJ/mol	Joback Method
hf	149.90	kJ/mol	Joback Method
hfus	50.00	kJ/mol	Joback Method
hvap	82.02	kJ/mol	Joback Method
log10ws	-10.45		Crippen Method
logp	8.267		Crippen Method
mcvol	299.360	ml/mol	McGowan Method
pc	1294.86	kPa	Joback Method
tb	885.14	K	Joback Method
tc	1104.59	K	Joback Method
tf	551.14	K	Joback Method
vc	1.179	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	934.53	J/molxK	885.14	Joback Method
cpg	1018.89	J/molxK	1068.01	Joback Method
cpg	1002.56	J/molxK	1031.44	Joback Method
cpg	986.12	J/molxK	994.86	Joback Method
cpg	969.41	J/molxK	958.29	Joback Method
cpg	952.26	J/molxK	921.71	Joback Method
cpg	1035.27	J/molxK	1104.59	Joback Method

dvisc	0.0007380	Paxs	885.14	Joback Method
dvisc	0.0008216	Paxs	829.47	Joback Method
dvisc	0.0009288	Paxs	773.81	Joback Method
dvisc	0.0010702	Paxs	718.14	Joback Method
dvisc	0.0012629	Paxs	662.47	Joback Method
dvisc	0.0015362	Paxs	606.81	Joback Method
dvisc	0.0019440	Paxs	551.14	Joback Method

## Sources

<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>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</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=C55682901&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C55682901&amp;Units=SI</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>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>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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