

Pyrene, 4-decyl-1,2,3,6,7,8-hexahydro-

Other names:	4-n-Decyl-(1,2,3,6,7,8-hexahydro)pyrene)
Inchi:	InChI=1S/C26H36/c1-2-3-4-5-6-7-8-9-12-22-19-23-15-10-13-20-17-18-21-14-11-16-24(2
InchiKey:	RJQGNYIKTOWQRO-UHFFFAOYSA-N
Formula:	C26H36
SMILES:	CCCCCCCCCc1cc2c3c(ccc4c3c1CCC4)CCC2
Mol. weight [g/mol]:	348.56
CAS:	56247-94-0

Physical Properties

Property code	Value	Unit	Source
gf	475.87	kJ/mol	Joback Method
hf	-23.44	kJ/mol	Joback Method
hfus	46.34	kJ/mol	Joback Method
hvap	81.14	kJ/mol	Joback Method
log10ws	-9.59		Crippen Method
logp	7.500		Crippen Method
mcvol	312.260	ml/mol	McGowan Method
pc	1199.79	kPa	Joback Method
tb	887.66	K	Joback Method
tc	1104.19	K	Joback Method
tf	345.65 ± 0.50	K	NIST Webbook
vc	1.222	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1022.68	J/molxK	887.66	Joback Method
cpg	1116.14	J/molxK	1068.10	Joback Method
cpg	1098.36	J/molxK	1032.01	Joback Method
cpg	1080.28	J/molxK	995.93	Joback Method
cpg	1061.73	J/molxK	959.84	Joback Method
cpg	1042.59	J/molxK	923.75	Joback Method
cpg	1133.77	J/molxK	1104.19	Joback Method
dvisc	0.0005809	Paxs	887.66	Joback Method

dvisc	0.0006617	Paxs	831.19	Joback Method
dvisc	0.0007682	Paxs	774.73	Joback Method
dvisc	0.0009130	Paxs	718.26	Joback Method
dvisc	0.0011176	Paxs	661.79	Joback Method
dvisc	0.0014206	Paxs	605.33	Joback Method
dvisc	0.0018971	Paxs	548.86	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.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=C56247940&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
mcvol:	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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