

Perylene, 3-hexyl-

Other names:	3-n-Hexylperylene 3-Hexylperylene
Inchi:	InChI=1S/C26H24/c1-2-3-4-5-9-18-16-17-24-22-14-7-11-19-10-6-13-21(25(19)22)23-15-
InchiKey:	TZZMLMCAA VPEBH-UHFFFAOYSA-N
Formula:	C26H24
SMILES:	CCCCCc1ccc2c3cccc4cccc(c5cccc1c52)c43
Mol. weight [g/mol]:	336.47
CAS:	7350-91-6

Physical Properties

Property code	Value	Unit	Source
gf	662.77	kJ/mol	Joback Method
hf	329.50	kJ/mol	Joback Method
hfus	46.63	kJ/mol	Joback Method
hvap	84.32	kJ/mol	Joback Method
log10ws	-10.58		Crippen Method
logp	7.860		Crippen Method
mvol	279.900	ml/mol	McGowan Method
pc	1539.08	kPa	Joback Method
tb	909.10	K	Joback Method
tc	1146.72	K	Joback Method
tf	414.65 ± 0.50	K	NIST Webbook
vc	1.101	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	856.26	J/mol×K	909.10	Joback Method
cpg	873.13	J/mol×K	948.70	Joback Method
cpg	889.73	J/mol×K	988.31	Joback Method
cpg	906.29	J/mol×K	1027.91	Joback Method
cpg	923.02	J/mol×K	1067.51	Joback Method
cpg	940.16	J/mol×K	1107.12	Joback Method
cpg	957.92	J/mol×K	1146.72	Joback Method

dvisc	0.0029547	Paxs	596.36	Joback Method
dvisc	0.0025594	Paxs	648.48	Joback Method
dvisc	0.0022648	Paxs	700.61	Joback Method
dvisc	0.0020384	Paxs	752.73	Joback Method
dvisc	0.0018598	Paxs	804.85	Joback Method
dvisc	0.0017159	Paxs	856.98	Joback Method
dvisc	0.0015978	Paxs	909.10	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=C7350916&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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