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)23-15-8
InchiKey: TZZMLMCAAVPEBH-UHFFFAOYSA-N
Formula: C26H24
SMILES: CCCCCCc1ccc2c3cccc4cccc(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
mcvol	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	m3/kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0015978	Pa×s	909.10	Joback Method
dvisc	0.0017159	Pa×s	856.98	Joback Method
dvisc	0.0018598	Pa×s	804.85	Joback Method
dvisc	0.0020384	Pa×s	752.73	Joback Method
dvisc	0.0022648	Pa×s	700.61	Joback Method
dvisc	0.0025594	Pa×s	648.48	Joback Method
dvisc	0.0029547	Pa×s	596.36	Joback Method

Sources

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
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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