

Indeno[1,2,3-cd]perylene

Inchi:	InChI=1S/C26H14/c1-2-8-17-16(7-1)20-11-13-22-18-9-3-5-15-6-4-10-19(24(15)18)23-14
InchiKey:	YTUILTQRCVAYNB-UHFFFAOYSA-N
Formula:	C26H14
SMILES:	c1ccc2c(c1)-c1ccc3c4cccc5cccc(c6ccc-2c1c36)c54
Mol. weight [g/mol]:	326.39
CAS:	101686-49-1

Physical Properties

Property code	Value	Unit	Source
gf	860.68	kJ/mol	Joback Method
hf	654.71	kJ/mol	Joback Method
hfus	43.26	kJ/mol	Joback Method
hvap	87.62	kJ/mol	Joback Method
log10ws	-11.56		Crippen Method
logp	7.385		Crippen Method
mcvol	245.280	ml/mol	McGowan Method
pc	2143.35	kPa	Joback Method
tb	944.34	K	Joback Method
tc	1213.26	K	Joback Method
tf	680.56	K	Joback Method
vc	0.976	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	717.27	J/mol×K	944.34	Joback Method
cpg	733.65	J/mol×K	989.16	Joback Method
cpg	751.03	J/mol×K	1033.98	Joback Method
cpg	769.83	J/mol×K	1078.80	Joback Method
cpg	790.49	J/mol×K	1123.62	Joback Method
cpg	813.43	J/mol×K	1168.44	Joback Method
cpg	839.08	J/mol×K	1213.26	Joback Method
dvisc	0.0154834	Pa×s	680.56	Joback Method
dvisc	0.0153618	Pa×s	724.52	Joback Method

dvisc	0.0152550	Pa×s	768.49	Joback Method
dvisc	0.0151603	Pa×s	812.45	Joback Method
dvisc	0.0150758	Pa×s	856.41	Joback Method
dvisc	0.0150001	Pa×s	900.38	Joback Method
dvisc	0.0149317	Pa×s	944.34	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C101686491&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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