Dibenz[e,ghi]indeno[1,2,3,4-pqra]perylene

Inchi: InChI=1S/C30H14/c1-2-6-19-18(5-1)21-12-10-15-8-9-16-11-13-22-20-7-3-4-17-14-23(19)
InchiKey: HSPVWCDUOWARPN-UHFFFAOYSA-N
Formula: C30H14
SMILES: c1cc2c3c(c1)cc1c4ccccc4c4ccc5ccc6ccc-2c2c6c5c4c1c32
Mol. weight [g/mol]: 374.43
CAS: 75449-96-6

Physical Properties

Property code	Value	Unit	Source
gf	1076.88	kJ/mol	Joback Method
hf	840.43	kJ/mol	Joback Method
hfus	52.84	kJ/mol	Joback Method
hvap	99.86	kJ/mol	Joback Method
log10ws	-13.78		Crippen Method
logp	8.615		Crippen Method
mcvol	271.320	ml/mol	McGowan Method
pc	1964.82	kPa	Joback Method
tb	1068.38	K	Joback Method
tc	1339.64	K	Joback Method
tf	828.64	K	Joback Method
vc	1.103	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	846.33	J/mol×K	1068.38	Joback Method
cpg	872.72	J/mol×K	1113.59	Joback Method
cpg	902.72	J/mol×K	1158.80	Joback Method
cpg	936.92	J/mol×K	1204.01	Joback Method
cpg	975.91	J/mol×K	1249.22	Joback Method
cpg	1020.28	J/mol×K	1294.43	Joback Method
cpg	1070.64	J/mol×K	1339.64	Joback Method
dvisc	0.2034947	Pa×s	828.64	Joback Method
dvisc	0.2138556	Pa×s	868.60	Joback Method

dvisc	0.2237645	Pa×s	908.55	Joback Method
dvisc	0.2332407	Pa×s	948.51	Joback Method
dvisc	0.2423043	Pa×s	988.47	Joback Method
dvisc	0.2509756	Pa×s	1028.42	Joback Method
dvisc	0.2592744	Pa×s	1068.38	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C75449966&Units=SI
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

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