Indeno[5,6,7,1-pqra]perylene

Inchi: InChI=1S/C24H12/c1-3-13-7-8-17-12-16-10-9-15-11-14-4-2-6-19-18(5-1)21(13)23(17)24(
InchiKey: WXJAUBFSNLBGKK-UHFFFAOYSA-N
Formula: C24H12
SMILES: C1=Cc2cc3ccc4cccc5c6cccc7cc1c2c(c76)c3c45
Mol. weight [g/mol]: 300.35
CAS: 96915-18-3

Physical Properties

Property code	Value	Unit	Source
gf	838.08	kJ/mol	Joback Method
hf	650.53	kJ/mol	Joback Method
hfus	41.06	kJ/mol	Joback Method
hvap	82.54	kJ/mol	Joback Method
log10ws	-10.18		Crippen Method
logp	6.812		Crippen Method
mcvol	221.400	ml/mol	McGowan Method
pc	2370.28	kPa	Joback Method
tb	890.88	K	Joback Method
tc	1154.51	K	Joback Method
tf	664.30	K	Joback Method
vc	0.893	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	625.52	J/mol×K	890.88	Joback Method
cpg	639.68	J/mol×K	934.82	Joback Method
cpg	654.66	J/mol×K	978.76	Joback Method
cpg	670.86	J/mol×K	1022.70	Joback Method
cpg	688.72	J/mol×K	1066.64	Joback Method
cpg	708.65	J/mol×K	1110.57	Joback Method
cpg	731.08	J/mol×K	1154.51	Joback Method
dvisc	0.0266312	Pa×s	664.30	Joback Method
dvisc	0.0275768	Pa×s	702.06	Joback Method

dvisc	0.0284544	Pa×s	739.83	Joback Method
dvisc	0.0292708	Pa×s	777.59	Joback Method
dvisc	0.0300317	Pa×s	815.35	Joback Method
dvisc	0.0307426	Pa×s	853.12	Joback Method
dvisc	0.0314079	Pa×s	890.88	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=C96915183&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

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