11H-Cyclopenta[ghi]perylene

Inchi: InChI=1S/C21H12/c1-3-12-7-9-14-11-15-10-8-13-4-2-6-17-16(5-1)18(12)20(14)21(15)19(
InchiKey: ASADLUKYSVGSHC-UHFFFAOYSA-N
Formula: C21H12
SMILES: c1cc2ccc3c4c5c(ccc6cccc(c(c1)c24)c65)C3
Mol. weight [g/mol]: 264.32
CAS: 83899-23-4

Physical Properties

Property code	Value	Unit	Source
gf	703.70	kJ/mol	Joback Method
hf	526.69	kJ/mol	Joback Method
hfus	34.56	kJ/mol	Joback Method
hvap	73.73	kJ/mol	Joback Method
log10ws	-8.45		Crippen Method
logp	5.641		Crippen Method
mcvol	198.590	ml/mol	McGowan Method
pc	2574.11	kPa	Joback Method
rinpol	470.53		NIST Webbook
rinpol	470.53		NIST Webbook
tb	802.55	K	Joback Method
tc	1062.21	K	Joback Method
tf	581.75	K	Joback Method
vc	0.795	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	543.75	J/mol×K	802.55	Joback Method
cpg	556.52	J/mol×K	845.83	Joback Method
cpg	569.14	J/mol×K	889.10	Joback Method
cpg	581.94	J/mol×K	932.38	Joback Method
cpg	595.27	J/mol×K	975.65	Joback Method
cpg	609.49	J/mol×K	1018.93	Joback Method
cpg	624.92	J/mol×K	1062.21	Joback Method

dvisc	0.0102272	Pa×s	581.75	Joback Method
dvisc	0.0103866	Pa×s	618.55	Joback Method
dvisc	0.0105301	Pa×s	655.35	Joback Method
dvisc	0.0106601	Pa×s	692.15	Joback Method
dvisc	0.0107783	Pa×s	728.95	Joback Method
dvisc	0.0108863	Pa×s	765.75	Joback Method
dvisc	0.0109853	Pa×s	802.55	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C83899234&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume