Pyracyclene

Inchi: InChI=1S/C14H8/c1-2-10-7-8-12-4-3-11-6-5-9(1)13(10)14(11)12/h1-8H
InchiKey: SFPDOMBOFWSXDM-UHFFFAOYSA-N
Formula: C14H8
SMILES: C1=Cc2ccc3c4c(ccc1c24)C=C3
Mol. weight [g/mol]: 176.21
CAS: 187-78-0

Physical Properties

Property code	Value	Unit	Source
gf	468.58	kJ/mol	Joback Method
hf	408.60	kJ/mol	NIST Webbook
hfs	325.40 ± 3.60	kJ/mol	NIST Webbook
hfus	22.29	kJ/mol	Joback Method
hsub	83.20	kJ/mol	NIST Webbook
hsub	83.20	kJ/mol	NIST Webbook
hvap	54.01	kJ/mol	Joback Method
log10ws	-4.98		Crippen Method
logp	3.807		Crippen Method
mcvol	134.580	ml/mol	McGowan Method
pc	3468.36	kPa	Joback Method
tb	597.90	K	Joback Method
tc	845.47	K	Joback Method
tf	409.66	K	Joback Method
vc	0.537	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	312.64	J/mol×K	597.90	Joback Method
cpg	324.15	J/mol×K	639.16	Joback Method
cpg	334.55	J/mol×K	680.42	Joback Method
cpg	344.04	J/mol×K	721.69	Joback Method
cpg	352.84	J/mol×K	762.95	Joback Method
cpg	361.15	J/mol×K	804.21	Joback Method

cpg	369.17	J/mol×K	845.47	Joback Method
dvisc	0.0021076	Pa×s	409.66	Joback Method
dvisc	0.0021058	Pa×s	441.03	Joback Method
dvisc	0.0021042	Pa×s	472.41	Joback Method
dvisc	0.0021028	Pa×s	503.78	Joback Method
dvisc	0.0021016	Pa×s	535.15	Joback Method
dvisc	0.0021005	Pa×s	566.53	Joback Method
dvisc	0.0020996	Pa×s	597.90	Joback Method
hsubt	82.00	kJ/mol	342.00	NIST Webbook

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=C187780&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
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
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