1-Keto-1,2,3,4-tetra-hydrophenanthrene

Inchi: InChI=1S/C14H12O/c15-14-7-3-6-12-11-5-2-1-4-10(11)8-9-13(12)14/h1-2,4-5,8-9H,3,6-7
InchiKey: KBARGPSSEIXDQU-UHFFFAOYSA-N
Formula: C14H12O
SMILES: O=C1CCCc2c1ccc1ccccc21
Mol. weight [g/mol]: 196.24
CAS: 573-22-8

Physical Properties

Property code	Value	Unit	Source
gf	200.57	kJ/mol	Joback Method
hf	21.65	kJ/mol	Joback Method
hfus	16.77	kJ/mol	Joback Method
hvap	56.64	kJ/mol	Joback Method
log10ws	-4.63		Crippen Method
logp	3.359		Crippen Method
mcvol	155.610	ml/mol	McGowan Method
pc	3110.57	kPa	Joback Method
tb	658.84	K	Joback Method
tc	920.33	K	Joback Method
tf	418.58	K	Joback Method
vc	0.591	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	401.91	J/mol×K	658.84	Joback Method
cpg	418.25	J/mol×K	702.42	Joback Method
cpg	433.30	J/mol×K	746.00	Joback Method
cpg	447.14	J/mol×K	789.59	Joback Method
cpg	459.88	J/mol×K	833.17	Joback Method
cpg	471.62	J/mol×K	876.75	Joback Method
cpg	482.44	J/mol×K	920.33	Joback Method

Sources

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=C573228&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
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