6H-Benzo[cd]pyren-6-one

Inchi: InChI=1S/C19H10O/c20-19-14-5-1-3-11-7-9-13-10-8-12-4-2-6-15(19)17(12)18(13)16(11)
InchiKey: CLIKSBRDCNSYNO-UHFFFAOYSA-N
Formula: C19H10O
SMILES: O=C1c2cccc3ccc4ccc5cccc1c5c4c23
Mol. weight [g/mol]: 254.28

Physical Properties

Property code	Value	Unit	Source
gf	473.01	kJ/mol	Joback Method
hf	296.13	kJ/mol	Joback Method
hfus	29.28	kJ/mol	Joback Method
hvap	71.86	kJ/mol	Joback Method
log10ws	-7.09		Crippen Method
logp	4.691		Crippen Method
mcvol	187.140	ml/mol	McGowan Method
pc	2805.41	kPa	Joback Method
rinpol	459.10		NIST Webbook
rinpol	453.90		NIST Webbook
rinpol	454.70		NIST Webbook
tb	808.35	K	Joback Method
tc	1077.23	K	Joback Method
tf	575.93	K	Joback Method
vc	0.739	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	512.78	J/mol×K	808.35	Joback Method
cpg	525.61	J/mol×K	853.16	Joback Method
cpg	537.89	J/mol×K	897.98	Joback Method
cpg	549.89	J/mol×K	942.79	Joback Method
cpg	561.84	J/mol×K	987.60	Joback Method
cpg	573.99	J/mol×K	1032.42	Joback Method
cpg	586.60	J/mol×K	1077.23	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R312557&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
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