7-benz[de]anthrene

Inchi: InChI=1S/C17H12O/c18-17-14-8-2-1-7-12(14)13-9-3-5-11-6-4-10-15(17)16(11)13/h1-8,1
InchiKey: YCDFFWNIVSTHMV-UHFFFAOYSA-N
Formula: C17H12O
SMILES: O=C1c2ccccc2C2CC=Cc3cccc1c32
Mol. weight [g/mol]: 232.28

Physical Properties

Property code	Value	Unit	Source
gf	336.87	kJ/mol	Joback Method
hf	136.62	kJ/mol	Joback Method
hfus	24.73	kJ/mol	Joback Method
hvap	64.48	kJ/mol	Joback Method
log10ws	-4.88		Crippen Method
logp	3.780		Crippen Method
mcvol	178.420	ml/mol	McGowan Method
pc	2787.66	kPa	Joback Method
rinpol	406.54		NIST Webbook
rinpol	406.54		NIST Webbook
rinpol	406.54		NIST Webbook
tb	737.52	K	Joback Method
tc	1003.88	K	Joback Method
tf	484.37	K	Joback Method
vc	0.688	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	491.65	J/mol×K	737.52	Joback Method
cpg	507.20	J/mol×K	781.91	Joback Method
cpg	521.53	J/mol×K	826.31	Joback Method
cpg	534.82	J/mol×K	870.70	Joback Method
cpg	547.22	J/mol×K	915.10	Joback Method
cpg	558.90	J/mol×K	959.49	Joback Method
cpg	570.03	J/mol×K	1003.88	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R15539&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