2,3,6,7-Dibenzofluorene

Inchi: InChI=1S/C21H12O/c22-21-19-11-15-7-3-1-5-13(15)9-17(19)18-10-14-6-2-4-8-16(14)12-
InchiKey: JZNRMTLFMCNYBH-UHFFFAOYSA-N
Formula: C21H12O
SMILES: O=C1c2cc3ccccc3cc2-c2cc3ccccc3cc21
Mol. weight [g/mol]: 280.32

Physical Properties

Property code	Value	Unit	Source
gf	495.61	kJ/mol	Joback Method
hf	300.31	kJ/mol	Joback Method
hfus	31.48	kJ/mol	Joback Method
hvap	76.95	kJ/mol	Joback Method
log10ws	-7.89		Crippen Method
logp	5.204		Crippen Method
mcvol	211.020	ml/mol	McGowan Method
pc	2515.07	kPa	Joback Method
rinpol	453.60		NIST Webbook
rinpol	455.00		NIST Webbook
tb	861.81	K	Joback Method
tc	1136.08	K	Joback Method
tf	592.19	K	Joback Method
vc	0.821	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	599.88	J/mol×K	861.81	Joback Method
cpg	613.90	J/mol×K	907.52	Joback Method
cpg	627.29	J/mol×K	953.23	Joback Method
cpg	640.31	J/mol×K	998.95	Joback Method
cpg	653.20	J/mol×K	1044.66	Joback Method
cpg	666.19	J/mol×K	1090.37	Joback Method
cpg	679.53	J/mol×K	1136.08	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R411535&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

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