5-Phenyl-10,11-dihydro-5H-dibenzo[a,d]cyclohept

Inchi: InChI=1S/C21H18O/c22-21(18-10-2-1-3-11-18)19-12-6-4-8-16(19)14-15-17-9-5-7-13-20(
InchiKey: CAIIMJUORNLXOK-UHFFFAOYSA-N
Formula: C21H18O
SMILES: OC1(c2ccccc2)c2ccccc2CCc2ccccc21
Mol. weight [g/mol]: 286.37

Physical Properties

Property code	Value	Unit	Source
gf	362.35	kJ/mol	Joback Method
hf	145.69	kJ/mol	Joback Method
hfus	27.42	kJ/mol	Joback Method
hvap	85.93	kJ/mol	Joback Method
log10ws	-5.38		Crippen Method
logp	4.069		Crippen Method
mcvol	230.480	ml/mol	McGowan Method
pc	2490.03	kPa	Joback Method
rinpol	2415.00		NIST Webbook
ripol	3507.00		NIST Webbook
tb	869.04	K	Joback Method
tc	1122.31	K	Joback Method
tf	533.39	K	Joback Method
vc	0.862	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	693.67	J/mol×K	869.04	Joback Method
cpg	710.77	J/mol×K	911.25	Joback Method
cpg	727.79	J/mol×K	953.46	Joback Method
cpg	745.03	J/mol×K	995.68	Joback Method
cpg	762.80	J/mol×K	1037.89	Joback Method
cpg	781.39	J/mol×K	1080.10	Joback Method
cpg	801.12	J/mol×K	1122.31	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R537716&Units=SI

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume