11-Phenyl-6,11-dihydrodibenzo[b,e]oxepin-11-ol

Inchi: InChI=1S/C20H16O2/c21-20(16-9-2-1-3-10-16)17-11-5-4-8-15(17)14-22-19-13-7-6-12-18
InchiKey: PBXKSEHHKZITRZ-UHFFFAOYSA-N
Formula: C20H16O2
SMILES: OC1(c2ccccc2)c2ccccc2COc2ccccc21
Mol. weight [g/mol]: 288.34

Physical Properties

Property code	Value	Unit	Source
gf	267.81	kJ/mol	Joback Method
hf	34.33	kJ/mol	Joback Method
hfus	32.80	kJ/mol	Joback Method
hvap	88.22	kJ/mol	Joback Method
log10ws	-5.20		Crippen Method
logp	3.863		Crippen Method
mcvol	222.260	ml/mol	McGowan Method
pc	2721.17	kPa	Joback Method
rinpol	2400.00		NIST Webbook
ripol	3548.00		NIST Webbook
tb	873.11	K	Joback Method
tc	1127.69	K	Joback Method
tf	548.69	K	Joback Method
vc	0.827	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	666.35	J/mol×K	873.11	Joback Method
cpg	682.45	J/mol×K	915.54	Joback Method
cpg	698.53	J/mol×K	957.97	Joback Method
cpg	714.91	J/mol×K	1000.40	Joback Method
cpg	731.87	J/mol×K	1042.83	Joback Method
cpg	749.72	J/mol×K	1085.26	Joback Method
cpg	768.76	J/mol×K	1127.69	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R537687&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume