Dibenz[b,e]oxepin-11(6H)-one

Other names:	6,11-Dihydrodibenz[b,e]oxepin-11-one
	6,11-Dihydrobenz[b,e]oxepin-11-one
Inchi:	InChI=1S/C14H10O2/c15-14-11-6-2-1-5-10(11)9-16-13-8-4-3-7-12(13)14/h1-8H,9H2
InchiKey:	YUSHFLBKQQILNV-UHFFFAOYSA-N
Formula:	C14H10O2
SMILES:	O=C1c2ccccc2COc2ccccc21
Mol. weight [g/mol]:	210.23
CAS:	4504-87-4

Physical Properties

Property code	Value	Unit	Source
gf	132.31	kJ/mol	Joback Method
hf	-58.73	kJ/mol	Joback Method
hfus	23.87	kJ/mol	Joback Method
hvap	61.61	kJ/mol	Joback Method
ie	9.63	eV	NIST Webbook
log10ws	-3.90		Crippen Method
logp	2.810		Crippen Method
mcvol	157.180	ml/mol	McGowan Method
pc	3299.15	kPa	Joback Method
tb	689.22	K	Joback Method
tc	957.55	K	Joback Method
tf	442.39	K	Joback Method
vc	0.590	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	409.57	J/mol×K	689.22	Joback Method
cpg	424.63	J/mol×K	733.94	Joback Method
cpg	438.38	J/mol×K	778.66	Joback Method
cpg	450.91	J/mol×K	823.39	Joback Method
cpg	462.32	J/mol×K	868.11	Joback Method
cpg	472.68	J/mol×K	912.83	Joback Method

cpg	482.08	J/mol×K	957.55	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4504874&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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume