

Indenone ethylene ketal

Inchi:	InChI=1S/C11H10O2/c1-2-4-10-9(3-1)5-6-11(10)12-7-8-13-11/h1-6H,7-8H2
InchiKey:	PGDSXGALIMPOPC-UHFFFAOYSA-N
Formula:	C11H10O2
SMILES:	C1=CC2(OCCO2)c2ccccc21
Mol. weight [g/mol]:	174.20
CAS:	6710-43-6

Physical Properties

Property code	Value	Unit	Source
gf	113.86	kJ/mol	Joback Method
hf	-76.51	kJ/mol	Joback Method
hfus	21.88	kJ/mol	Joback Method
hvap	51.49	kJ/mol	Joback Method
log10ws	-2.14		Crippen Method
logp	1.913		Crippen Method
mcvol	127.810	ml/mol	McGowan Method
pc	4021.02	kPa	Joback Method
tb	558.46	K	Joback Method
tc	813.42	K	Joback Method
tf	367.07	K	Joback Method
vc	0.476	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	312.16	J/molxK	558.46	Joback Method
cpg	327.03	J/molxK	600.95	Joback Method
cpg	340.48	J/molxK	643.45	Joback Method
cpg	352.78	J/molxK	685.94	Joback Method
cpg	364.20	J/molxK	728.43	Joback Method
cpg	375.03	J/molxK	770.93	Joback Method
cpg	385.54	J/molxK	813.42	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6710436&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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