Benzalphthalide

Other names:	3-Benzalphthalide
	1(3H)-Isobenzofuranone, 3-(phenylmethylene)-
	Phthalide, 3-benzylidene-
	3-Benzylidenephthalide
	Benzalphthalid
Inchi:	InChI=1S/C15H10O2/c16-15-13-9-5-4-8-12(13)14(17-15)10-11-6-2-1-3-7-11/h1-10H/b14
InchiKey:	YRTPZXMEBGTPLM-UVTDQMKNSA-N
Formula:	C15H10O2
SMILES:	O=C1OC(=Cc2ccccc2)c2ccccc21
Mol. weight [g/mol]:	222.24
CAS:	575-61-1

Physical Properties

Property code	Value	Unit	Source
gf	195.82	kJ/mol	Joback Method
hf	8.13	kJ/mol	Joback Method
hfus	27.18	kJ/mol	Joback Method
hvap	63.96	kJ/mol	Joback Method
log10ws	-4.29		Crippen Method
logp	3.355		Crippen Method
mcvol	166.970	ml/mol	McGowan Method
pc	3110.57	kPa	Joback Method
tb	713.76	K	Joback Method
tc	982.37	K	Joback Method
tf	451.50	K	Joback Method
vc	0.628	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	436.74	J/mol×K	713.76	Joback Method
cpg	451.34	J/mol×K	758.53	Joback Method
cpg	464.68	J/mol×K	803.30	Joback Method
cpg	476.84	J/mol×K	848.07	Joback Method

cpg	487.94	J/mol×K	892.84	Joback Method
cpg	498.09	J/mol×K	937.61	Joback Method
cpg	507.40	J/mol×K	982.37	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C575611&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