

7-Benzoyloxybicyclo[2.2.1]hepta-2,5-diene

Other names:	7-Benzoyloxynorbornadiene 7-Norbornadienyl benzoate
Inchi:	InChI=1S/C14H12O2/c15-14(12-4-2-1-3-5-12)16-13-10-6-7-11(13)9-8-10/h1-11,13H
InchiKey:	NTELHPJRBBSUIJ-UHFFFAOYSA-N
Formula:	C14H12O2
SMILES:	O=C(OC1C2C=CC1C=C2)c1ccccc1
Mol. weight [g/mol]:	212.24
CAS:	4796-68-3

Physical Properties

Property code	Value	Unit	Source
gf	107.10	kJ/mol	Joback Method
hf	-105.90	kJ/mol	Joback Method
hfus	26.53	kJ/mol	Joback Method
hvap	58.46	kJ/mol	Joback Method
log10ws	-3.35		Crippen Method
logp	2.584		Crippen Method
mcvol	161.480	ml/mol	McGowan Method
pc	2887.40	kPa	Joback Method
tb	634.09	K	Joback Method
tc	874.61	K	Joback Method
tf	375.76	K	Joback Method
vc	0.613	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	425.21	J/mol×K	634.09	Joback Method
cpg	495.66	J/mol×K	834.52	Joback Method
cpg	483.83	J/mol×K	794.44	Joback Method
cpg	470.96	J/mol×K	754.35	Joback Method
cpg	456.98	J/mol×K	714.26	Joback Method
cpg	441.76	J/mol×K	674.18	Joback Method
cpg	506.58	J/mol×K	874.61	Joback Method

dvisc	0.0008988	Pa×s	634.09	Joback Method
dvisc	0.0009823	Pa×s	591.03	Joback Method
dvisc	0.0010886	Pa×s	547.98	Joback Method
dvisc	0.0012277	Pa×s	504.92	Joback Method
dvisc	0.0014160	Pa×s	461.87	Joback Method
dvisc	0.0016818	Pa×s	418.81	Joback Method
dvisc	0.0020778	Pa×s	375.76	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	400.50 ± 2.50	K	0.20	NIST Webbook

Sources

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=C4796683&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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
tbrp:	Boiling point at reduced pressure

tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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