7-Norbornadienyl benzoate

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]: 212.25

Physical Properties

Property code	Value	Unit	Source
af	0.4533		Cheméo Relay (1.0)
gf	107.10	kJ/mol	Joback Method
hf	-60.45	kJ/mol	Cheméo Relay (1.0)
hfus	26.53	kJ/mol	Joback Method
hvap	83.24	kJ/mol	Cheméo Relay (1.0)
ie	8.74	eV	Cheméo Relay (1.0)
log10ws	-3.52		Cheméo Relay (1.0)
logp	2.584		Crippen Method
mcvol	161.480	ml/mol	McGowan Method
pc	2887.40	kPa	Joback Method
tb	550.16	K	Cheméo Relay (1.0)
tc	812.40	K	Cheméo Relay (1.0)
tf	335.41	K	Cheméo Relay (1.0)
vc	0.590	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

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

cpg	506.58	J/mol×K	874.61	Joback Method
dvisc	0.0020778	Pa×s	375.76	Joback Method
dvisc	0.0016818	Pa×s	418.81	Joback Method
dvisc	0.0014160	Pa×s	461.87	Joback Method
dvisc	0.0012277	Pa×s	504.92	Joback Method
dvisc	0.0010886	Pa×s	547.98	Joback Method
dvisc	0.0009823	Pa×s	591.03	Joback Method
dvisc	0.0008988	Pa×s	634.09	Joback Method

Pressure Dependent Properties

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

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C4796683&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):

Legend

af: Acentric Factor
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
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume