

1-Hexen-3-ol, benzoate

Inchi:	InChI=1S/C13H16O2/c1-3-8-12(4-2)15-13(14)11-9-6-5-7-10-11/h4-7,9-10,12H,2-3,8H2,1
InchiKey:	PWEVLLZPVANVOL-UHFFFAOYSA-N
Formula:	C13H16O2
SMILES:	<chem>C=CC(CCC)OC(=O)c1ccccc1</chem>
Mol. weight [g/mol]:	204.26

Physical Properties

Property code	Value	Unit	Source
gf	22.47	kJ/mol	Joback Method
hf	-199.77	kJ/mol	Joback Method
hfus	21.45	kJ/mol	Joback Method
hvap	54.91	kJ/mol	Joback Method
log10ws	-3.77		Crippen Method
logp	3.198		Crippen Method
mcvol	173.410	ml/mol	McGowan Method
pc	2405.28	kPa	Joback Method
rinpol	1573.00		NIST Webbook
rinpol	1573.00		NIST Webbook
tb	596.05	K	Joback Method
tc	807.15	K	Joback Method
tf	318.09	K	Joback Method
vc	0.654	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	422.73	J/molxK	596.05	Joback Method
cpg	438.31	J/molxK	631.23	Joback Method
cpg	452.94	J/molxK	666.42	Joback Method
cpg	466.67	J/molxK	701.60	Joback Method
cpg	479.52	J/molxK	736.78	Joback Method
cpg	491.52	J/molxK	771.97	Joback Method
cpg	502.71	J/molxK	807.15	Joback Method
dvisc	0.0026678	Paxs	318.09	Joback Method

dvisc	0.0012441	Paxs	364.42	Joback Method
dvisc	0.0006891	Paxs	410.74	Joback Method
dvisc	0.0004302	Paxs	457.07	Joback Method
dvisc	0.0002929	Paxs	503.40	Joback Method
dvisc	0.0002128	Paxs	549.72	Joback Method
dvisc	0.0001625	Paxs	596.05	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R579963&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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