3-Hexen-1-ol benzoate

Other names: (E)-3-Hexenyl benzoate
Inchi: InChI=1S/C13H16O2/c1-2-3-4-8-11-15-13(14)12-9-6-5-7-10-12/h3-7,9-10H,2,8,11H2,1H
InchiKey: BCOXBEHFBZOJJZ-ARJAWSKDSA-N
Formula: C13H16O2
SMILES: CCC=CCCOC(=O)c1ccccc1
Mol. weight [g/mol]: 204.26

Physical Properties

Property code	Value	Unit	Source
gf	17.29	kJ/mol	Joback Method
hf	-202.70	kJ/mol	Joback Method
hfus	26.46	kJ/mol	Joback Method
hvap	55.92	kJ/mol	Joback Method
log10ws	-3.66		Crippen Method
logp	3.200		Crippen Method
mcvol	173.410	ml/mol	McGowan Method
pc	2410.00	kPa	Joback Method
rinpol	1540.00		NIST Webbook
rinpol	1553.00		NIST Webbook
rinpol	1585.00		NIST Webbook
rinpol	1541.00		NIST Webbook
rinpol	1545.00		NIST Webbook
rinpol	1535.00		NIST Webbook
rinpol	1546.00		NIST Webbook
rinpol	1549.00		NIST Webbook
rinpol	1544.00		NIST Webbook
rinpol	1536.00		NIST Webbook
rinpol	1553.00		NIST Webbook
rinpol	1540.00		NIST Webbook
rinpol	1536.00		NIST Webbook
rinpol	1540.00		NIST Webbook
rinpol	1549.00		NIST Webbook
ripol	2089.00		NIST Webbook
ripol	2101.00		NIST Webbook
ripol	2095.00		NIST Webbook
ripol	2120.00		NIST Webbook
ripol	2069.00		NIST Webbook

ripol	2051.00		NIST Webbook
ripol	2046.00		NIST Webbook
ripol	2115.00		NIST Webbook
ripol	2100.00		NIST Webbook
ripol	2083.00		NIST Webbook
ripol	2069.00		NIST Webbook
ripol	2088.00		NIST Webbook
tb	603.97	K	Joback Method
tc	815.36	K	Joback Method
tf	329.77	K	Joback Method
vc	0.659	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	423.08	J/mol×K	603.97	Joback Method
cpg	438.38	J/mol×K	639.20	Joback Method
cpg	452.75	J/mol×K	674.43	Joback Method
cpg	466.22	J/mol×K	709.66	Joback Method
cpg	478.84	J/mol×K	744.90	Joback Method
cpg	490.65	J/mol×K	780.13	Joback Method
cpg	501.68	J/mol×K	815.36	Joback Method
dvisc	0.0019948	Pa×s	329.77	Joback Method
dvisc	0.0009848	Pa×s	375.47	Joback Method
dvisc	0.0005667	Pa×s	421.17	Joback Method
dvisc	0.0003633	Pa×s	466.87	Joback Method
dvisc	0.0002522	Pa×s	512.57	Joback Method
dvisc	0.0001858	Pa×s	558.27	Joback Method
dvisc	0.0001434	Pa×s	603.97	Joback Method

Sources

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

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U132066&Units=SI

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume