Benzoic acid, heptyl ester

Other names:	n-Heptyl benzoate
	heptyl benzoate
Inchi:	InChI=1S/C14H20O2/c1-2-3-4-5-9-12-16-14(15)13-10-7-6-8-11-13/h6-8,10-11H,2-5,9,12
InchiKey:	UMFTYCUYCNMERS-UHFFFAOYSA-N
Formula:	C14H20O2
SMILES:	CCCCCCCOC(=O)c1ccccc1
Mol. weight [g/mol]:	220.31
CAS:	7155-12-6

Physical Properties

Property code	Value	Unit	Source
gf	-54.51	kJ/mol	Joback Method
hf	-340.56	kJ/mol	Joback Method
hfus	28.84	kJ/mol	Joback Method
hvap	58.19	kJ/mol	Joback Method
log10ws	-4.23		Crippen Method
logp	3.814		Crippen Method
mcvol	191.800	ml/mol	McGowan Method
pc	2094.58	kPa	Joback Method
rinpol	1657.00		NIST Webbook
rinpol	1662.00		NIST Webbook
rinpol	1653.00		NIST Webbook
rinpol	1668.00		NIST Webbook
rinpol	1651.00		NIST Webbook
rinpol	1704.00		NIST Webbook
rinpol	1654.00		NIST Webbook
rinpol	1646.00		NIST Webbook
rinpol	1638.00		NIST Webbook
rinpol	1673.00		NIST Webbook
rinpol	1683.00		NIST Webbook
rinpol	1665.00		NIST Webbook
rinpol	1682.49		NIST Webbook
rinpol	1660.00		NIST Webbook
rinpol	1673.00		NIST Webbook
rinpol	1704.00		NIST Webbook
rinpol	1683.00		NIST Webbook
rinpol	1663.10		NIST Webbook

rinpol	1672.00		NIST Webbook
rinpol	1665.00		NIST Webbook
rinpol	1657.00		NIST Webbook
rinpol	1657.00		NIST Webbook
rinpol	1660.00		NIST Webbook
rinpol	1670.00		NIST Webbook
rinpol	1663.10		NIST Webbook
ripol	2184.00		NIST Webbook
ripol	2184.00		NIST Webbook
ripol	2169.00		NIST Webbook
ripol	2198.00		NIST Webbook
ripol	2184.00		NIST Webbook
ripol	2151.00		NIST Webbook
ripol	2217.00		NIST Webbook
ripol	2217.00		NIST Webbook
ripol	2158.00		NIST Webbook
ripol	2142.00		NIST Webbook
ripol	2176.00		NIST Webbook
ripol	2151.00		NIST Webbook
ripol	2207.00		NIST Webbook
ripol	2174.00		NIST Webbook
ripol	2199.00		NIST Webbook
tb	622.69	K	Joback Method
tc	822.76	K	Joback Method
tf	346.12	K	Joback Method
vc	0.736	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	494.13	J/mol×K	622.69	Joback Method
cpg	510.47	J/mol×K	656.04	Joback Method
cpg	525.89	J/mol×K	689.38	Joback Method
cpg	540.43	J/mol×K	722.73	Joback Method
cpg	554.11	J/mol×K	756.07	Joback Method
cpg	566.96	J/mol×K	789.42	Joback Method
cpg	579.01	J/mol×K	822.76	Joback Method
dvisc	0.0020543	Pa×s	346.12	Joback Method
dvisc	0.0010310	Pa×s	392.21	Joback Method
dvisc	0.0005982	Pa×s	438.31	Joback Method
dvisc	0.0003849	Pa×s	484.40	Joback Method

dvisc	0.0002674	Pa×s	530.50	Joback Method
dvisc	0.0001969	Pa×s	576.60	Joback Method
dvisc	0.0001517	Pa×s	622.69	Joback Method

Sources

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=C7155126&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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