Benzoic acid, hexyl ester

Other names:	Benzoic acid n-hexyl ester
	Hexylester kyseliny benzoove
	hexyl benzoate
	n-Hexyl benzoate
Inchi:	InChI=1S/C13H18O2/c1-2-3-4-8-11-15-13(14)12-9-6-5-7-10-12/h5-7,9-10H,2-4,8,11H2,1
InchiKey:	UUGLJVMIFJNVFH-UHFFFAOYSA-N
Formula:	C13H18O2
SMILES:	CCCCCCOC(=O)c1ccccc1
Mol. weight [g/mol]:	206.28
CAS:	6789-88-4

Physical Properties

Property code	Value	Unit	Source
gf	-62.93	kJ/mol	Joback Method
hf	-319.92	kJ/mol	Joback Method
hfus	26.25	kJ/mol	Joback Method
hvap	55.96	kJ/mol	Joback Method
log10ws	-3.81		Crippen Method
logp	3.424		Crippen Method
mcvol	177.710	ml/mol	McGowan Method
pc	1980.00	kPa	Critical Point Measurements for n-Alkyl Benzoates (C8 to C13)
rinpol	1568.00		NIST Webbook
rinpol	1572.00		NIST Webbook
rinpol	1558.00		NIST Webbook
rinpol	1557.00		NIST Webbook
rinpol	1573.00		NIST Webbook
rinpol	1549.00		NIST Webbook
rinpol	1556.00		NIST Webbook
rinpol	1579.00		NIST Webbook
rinpol	1579.00		NIST Webbook
rinpol	1551.00		NIST Webbook
rinpol	1551.00		NIST Webbook
rinpol	1599.00		NIST Webbook
rinpol	1576.50		NIST Webbook
rinpol	1574.00		NIST Webbook
rinpol	1548.30		NIST Webbook

rinpol	1547.10	NIST Webbook
rinpol	1557.40	NIST Webbook
rinpol	1565.30	NIST Webbook
rinpol	1550.50	NIST Webbook
rinpol	1556.00	NIST Webbook
rinpol	1559.28	NIST Webbook
rinpol	1551.00	NIST Webbook
rinpol	1565.00	NIST Webbook
rinpol	1550.00	NIST Webbook
rinpol	1558.00	NIST Webbook
rinpol	1565.00	NIST Webbook
rinpol	1581.00	NIST Webbook
rinpol	1580.00	NIST Webbook
rinpol	1585.00	NIST Webbook
rinpol	1545.00	NIST Webbook
rinpol	1561.00	NIST Webbook
rinpol	1576.00	NIST Webbook
rinpol	1589.00	NIST Webbook
rinpol	1560.00	NIST Webbook
rinpol	1576.00	NIST Webbook
rinpol	1593.00	NIST Webbook
rinpol	1577.00	NIST Webbook
rinpol	1540.00	NIST Webbook
rinpol	1551.90	NIST Webbook
rinpol	1542.70	NIST Webbook
rinpol	1552.80	NIST Webbook
rinpol	1552.20	NIST Webbook
rinpol	1556.50	NIST Webbook
rinpol	1549.00	NIST Webbook
rinpol	1580.00	NIST Webbook
rinpol	1581.00	NIST Webbook
rinpol	1579.00	NIST Webbook
rinpol	1580.00	NIST Webbook
rinpol	1555.00	NIST Webbook
rinpol	1551.00	NIST Webbook
rinpol	1599.00	NIST Webbook
rinpol	1557.40	NIST Webbook
rinpol	1551.00	NIST Webbook
rinpol	1556.00	NIST Webbook
rinpol	1595.76	NIST Webbook
rinpol	1575.95	NIST Webbook
rinpol	1558.00	NIST Webbook
rinpol	1566.00	NIST Webbook
ripol	2093.00	NIST Webbook

ripol	2073.00		NIST Webbook
ripol	2081.00		NIST Webbook
ripol	2069.00		NIST Webbook
ripol	2046.00		NIST Webbook
ripol	2070.00		NIST Webbook
ripol	2033.00		NIST Webbook
ripol	2051.00		NIST Webbook
ripol	2069.00		NIST Webbook
ripol	2056.00		NIST Webbook
ripol	2028.00		NIST Webbook
ripol	2076.00		NIST Webbook
ripol	2095.00		NIST Webbook
ripol	2074.00		NIST Webbook
ripol	2056.00		NIST Webbook
ripol	2066.00		NIST Webbook
ripol	2095.00		NIST Webbook
ripol	2096.00		NIST Webbook
ripol	2096.00		NIST Webbook
ripol	2095.00		NIST Webbook
ripol	2097.00		NIST Webbook
ripol	2107.00		NIST Webbook
tb	599.81	K	Joback Method
tc	802.73	K	Joback Method
tf	334.85	K	Joback Method
vc	0.679	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	443.32	J/mol×K	599.81	Joback Method
cpg	459.12	J/mol×K	633.63	Joback Method
cpg	474.04	J/mol×K	667.45	Joback Method
cpg	488.11	J/mol×K	701.27	Joback Method
cpg	501.35	J/mol×K	735.09	Joback Method
cpg	513.77	J/mol×K	768.91	Joback Method
cpg	525.42	J/mol×K	802.73	Joback Method
dvisc	0.0021584	Pa×s	334.85	Joback Method
dvisc	0.0011004	Pa×s	379.01	Joback Method
dvisc	0.0006457	Pa×s	423.17	Joback Method
dvisc	0.0004190	Pa×s	467.33	Joback Method
dvisc	0.0002930	Pa×s	511.49	Joback Method

dvisc	0.0002169	Pa×s	555.65	Joback Method
dvisc	0.0001678	Pa×s	599.81	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Critical Point Measurements for n-Alkyl Benzoates (C8 to C13):	https://www.doi.org/10.1021/je700049s
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=C6789884&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