Benzoic acid, 3-chloro, hexyl ester

Other names: Benzoic acid, 3-chloro, hexyl ester
Inchi: InChI=1S/C13H17ClO2/c1-2-3-4-5-9-16-13(15)11-7-6-8-12(14)10-11/h6-8,10H,2-5,9H2,1
InchiKey: WIOHDOZCKINPRO-UHFFFAOYSA-N
Formula: C13H17ClO2
SMILES: CCCCCCOC(=O)c1cccc(Cl)c1
Mol. weight [g/mol]: 240.73

Physical Properties

Property code	Value	Unit	Source
af	0.6803		Cheméo Relay (1.0)
hf	-421.30	kJ/mol	Cheméo Relay (1.0)
hfus	30.06	kJ/mol	Joback Method
hvap	76.51	kJ/mol	Cheméo Relay (1.0)
ie	9.21	eV	Cheméo Relay (1.0)
log10ws	-5.24		Cheméo Relay (1.0)
logp	4.077		Crippen Method
mcvol	189.950	ml/mol	McGowan Method
pc	2181.56	kPa	Joback Method
rinpol	1723.00		NIST Webbook
rinpol	1756.00		NIST Webbook
rinpol	1714.00		NIST Webbook
rinpol	1722.00		NIST Webbook
rinpol	1712.00		NIST Webbook
rinpol	1731.00		NIST Webbook
rinpol	1756.00		NIST Webbook
rinpol	1732.00		NIST Webbook
rinpol	1714.00		NIST Webbook
ripol	2251.00		NIST Webbook
ripol	2244.00		NIST Webbook
ripol	2251.00		NIST Webbook
ripol	2264.00		NIST Webbook
ripol	2225.00		NIST Webbook
ripol	2264.00		NIST Webbook
ripol	2295.00		NIST Webbook
ripol	2263.00		NIST Webbook
tb	573.42	K	Cheméo Relay (1.0)
tc	772.15	K	Cheméo Relay (1.0)

tf	259.10	K	Cheméo Relay (1.0)
vc	0.701	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	471.36	J/mol×K	642.22	Joback Method
cpg	485.98	J/mol×K	676.82	Joback Method
cpg	499.75	J/mol×K	711.43	Joback Method
cpg	512.68	J/mol×K	746.03	Joback Method
cpg	524.81	J/mol×K	780.63	Joback Method
cpg	536.14	J/mol×K	815.23	Joback Method
cpg	546.71	J/mol×K	849.84	Joback Method
dvisc	0.0014793	Pa×s	377.29	Joback Method
dvisc	0.0008357	Pa×s	421.45	Joback Method
dvisc	0.0005262	Pa×s	465.60	Joback Method
dvisc	0.0003589	Pa×s	509.75	Joback Method
dvisc	0.0002602	Pa×s	553.91	Joback Method
dvisc	0.0001978	Pa×s	598.07	Joback Method
dvisc	0.0001562	Pa×s	642.22	Joback Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U373563&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):

Legend

af: Acentric Factor

cpg: Ideal gas heat capacity

dvisc: Dynamic viscosity

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
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