(E)-Hex-3-enyl 3-chlorobenzoate

Other names: Benzoic acid, 3-chloro, (E)-3-hexenyl ester
Inchi: InChI=1S/C13H15ClO2/c1-2-3-4-5-9-16-13(15)11-7-6-8-12(14)10-11/h3-4,6-8,10H,2,5,9H
InchiKey: PSTUDEYXVHRFJN-ONEGZZNKSA-N
Formula: C13H15ClO2
SMILES: CCC=CCCOC(=O)c1cccc(Cl)c1
Mol. weight [g/mol]: 238.71

Physical Properties

Property code	Value	Unit	Source
gf	-4.27	kJ/mol	Joback Method
hf	-229.91	kJ/mol	Joback Method
hfus	30.26	kJ/mol	Joback Method
hvap	60.97	kJ/mol	Joback Method
log10ws	-4.35		Crippen Method
logp	3.853		Crippen Method
mcvol	185.650	ml/mol	McGowan Method
pc	2291.52	kPa	Joback Method
rinpol	1702.00		NIST Webbook
rinpol	1691.00		NIST Webbook
rinpol	1712.00		NIST Webbook
rinpol	1739.00		NIST Webbook
rinpol	1704.00		NIST Webbook
rinpol	1696.00		NIST Webbook
rinpol	1739.00		NIST Webbook
rinpol	1686.00		NIST Webbook
ripol	2312.00		NIST Webbook
ripol	2282.00		NIST Webbook
ripol	2293.00		NIST Webbook
ripol	2255.00		NIST Webbook
ripol	2276.00		NIST Webbook
ripol	2296.00		NIST Webbook
ripol	2255.00		NIST Webbook
tb	646.38	K	Joback Method
tc	862.28	K	Joback Method
tf	372.21	K	Joback Method
vc	0.709	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	449.70	J/mol×K	646.38	Joback Method
cpg	463.75	J/mol×K	682.36	Joback Method
cpg	476.91	J/mol×K	718.35	Joback Method
cpg	489.23	J/mol×K	754.33	Joback Method
cpg	500.74	J/mol×K	790.31	Joback Method
cpg	511.47	J/mol×K	826.29	Joback Method
cpg	521.47	J/mol×K	862.28	Joback Method
dvisc	0.0013603	Pa×s	372.21	Joback Method
dvisc	0.0007487	Pa×s	417.91	Joback Method
dvisc	0.0004636	Pa×s	463.60	Joback Method
dvisc	0.0003128	Pa×s	509.30	Joback Method
dvisc	0.0002252	Pa×s	554.99	Joback Method
dvisc	0.0001705	Pa×s	600.68	Joback Method
dvisc	0.0001342	Pa×s	646.38	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=U373561&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