Pent-4-enyl 3-chlorobenzoate

Other names: Benzoic acid, 3-chloro, 4-pentenyl ester
Inchi: InChI=1S/C12H13ClO2/c1-2-3-4-8-15-12(14)10-6-5-7-11(13)9-10/h2,5-7,9H,1,3-4,8H2
InchiKey: RDVBXOHTBOIYCP-UHFFFAOYSA-N
Formula: C12H13ClO2
SMILES: C=CCCCOC(=O)c1cccc(Cl)c1
Mol. weight [g/mol]: 224.68

Physical Properties

Property code	Value	Unit	Source
gf	-5.07	kJ/mol	Joback Method
hf	-201.06	kJ/mol	Joback Method
hfus	26.19	kJ/mol	Joback Method
hvap	58.12	kJ/mol	Joback Method
log10ws	-3.93		Crippen Method
logp	3.463		Crippen Method
mcvol	171.560	ml/mol	McGowan Method
pc	2492.52	kPa	Joback Method
rinpol	1604.00		NIST Webbook
rinpol	1642.00		NIST Webbook
rinpol	1606.00		NIST Webbook
rinpol	1595.00		NIST Webbook
rinpol	1612.00		NIST Webbook
rinpol	1642.00		NIST Webbook
rinpol	1593.00		NIST Webbook
rinpol	1593.00		NIST Webbook
rinpol	1612.00		NIST Webbook
ripol	2208.00		NIST Webbook
ripol	2187.00		NIST Webbook
ripol	2239.00		NIST Webbook
ripol	2187.00		NIST Webbook
ripol	2219.00		NIST Webbook
ripol	2208.00		NIST Webbook
ripol	2239.00		NIST Webbook
ripol	2229.00		NIST Webbook
tb	616.02	K	Joback Method
tc	831.07	K	Joback Method
tf	364.26	K	Joback Method

vc	0.653	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	400.01	J/mol×K	616.02	Joback Method
cpg	413.37	J/mol×K	651.86	Joback Method
cpg	425.91	J/mol×K	687.70	Joback Method
cpg	437.64	J/mol×K	723.55	Joback Method
cpg	448.61	J/mol×K	759.39	Joback Method
cpg	458.82	J/mol×K	795.23	Joback Method
cpg	468.31	J/mol×K	831.07	Joback Method
dvisc	0.0015161	Pa×s	364.26	Joback Method
dvisc	0.0008854	Pa×s	406.22	Joback Method
dvisc	0.0005718	Pa×s	448.18	Joback Method
dvisc	0.0003980	Pa×s	490.14	Joback Method
dvisc	0.0002933	Pa×s	532.10	Joback Method
dvisc	0.0002260	Pa×s	574.06	Joback Method
dvisc	0.0001805	Pa×s	616.02	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=U373560&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

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