

But-3-enyl 3-chlorobenzoate

Other names:	Benzoic acid, 3-chloro, 3-butenyl ester
Inchi:	InChI=1S/C11H11ClO2/c1-2-3-7-14-11(13)9-5-4-6-10(12)8-9/h2,4-6,8H,1,3,7H2
InchiKey:	WHZYVADNTJUCRC-UHFFFAOYSA-N
Formula:	C11H11ClO2
SMILES:	<chem>C=CCOC(=O)c1cccc(Cl)c1</chem>
Mol. weight [g/mol]:	210.66

Physical Properties

Property code	Value	Unit	Source
gf	-13.49	kJ/mol	Joback Method
hf	-180.42	kJ/mol	Joback Method
hfus	23.60	kJ/mol	Joback Method
hvap	55.89	kJ/mol	Joback Method
log10ws	-3.51		Crippen Method
logp	3.073		Crippen Method
mcvol	157.470	ml/mol	McGowan Method
pc	2749.78	kPa	Joback Method
ripol	1494.00		NIST Webbook
ripol	1529.00		NIST Webbook
ripol	1505.00		NIST Webbook
ripol	1498.00		NIST Webbook
ripol	1488.00		NIST Webbook
ripol	1485.00		NIST Webbook
ripol	1529.00		NIST Webbook
ripol	1499.00		NIST Webbook
ripol	1488.00		NIST Webbook
ripol	2119.00		NIST Webbook
ripol	2119.00		NIST Webbook
ripol	2101.00		NIST Webbook
ripol	2082.00		NIST Webbook
ripol	2104.00		NIST Webbook
ripol	2088.00		NIST Webbook
ripol	2122.00		NIST Webbook
ripol	2082.00		NIST Webbook
tb	593.14	K	Joback Method
tc	811.98	K	Joback Method
tf	352.99	K	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	352.26	J/molxK	593.14	Joback Method
cpg	364.87	J/molxK	629.61	Joback Method
cpg	376.70	J/molxK	666.09	Joback Method
cpg	387.76	J/molxK	702.56	Joback Method
cpg	398.08	J/molxK	739.03	Joback Method
cpg	407.69	J/molxK	775.50	Joback Method
cpg	416.61	J/molxK	811.98	Joback Method
dvisc	0.0015687	Paxs	352.99	Joback Method
dvisc	0.0009325	Paxs	393.01	Joback Method
dvisc	0.0006103	Paxs	433.04	Joback Method
dvisc	0.0004291	Paxs	473.06	Joback Method
dvisc	0.0003187	Paxs	513.09	Joback Method
dvisc	0.0002472	Paxs	553.12	Joback Method
dvisc	0.0001984	Paxs	593.14	Joback Method

Sources

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=U373546&Units=SI>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Crippen Method:

https://www.chemeo.com/doc/models/crippen_log10ws

Joback Method:

https://en.wikipedia.org/wiki/Joback_method

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

h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀w_s:	Log ₁₀ of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mc_{vol}:	McGowan's characteristic volume
p_c:	Critical Pressure
r_{inpol}:	Non-polar retention indices
r_{ipol}:	Polar retention indices
t_b:	Normal Boiling Point Temperature
t_c:	Critical Temperature
t_f:	Normal melting (fusion) point
v_c:	Critical Volume

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