(E)-But-2-enyl 3-chlorobenzoate

Other names: Benzoic acid, 3-chloro, (E)-2-butenyl ester
Inchi: InChI=1S/C11H11ClO2/c1-2-3-7-14-11(13)9-5-4-6-10(12)8-9/h2-6,8H,7H2,1H3/b3-2+
InchiKey: YSMHCWQQKGGAQR-NSCUHMNNSA-N
Formula: C11H11ClO2
SMILES: CC=CCOC(=O)c1cccc(Cl)c1
Mol. weight [g/mol]: 210.66

Physical Properties

Property code	Value	Unit	Source
gf	-21.11	kJ/mol	Joback Method
hf	-188.63	kJ/mol	Joback Method
hfus	25.08	kJ/mol	Joback Method
hvap	56.52	kJ/mol	Joback Method
log10ws	-3.51		Crippen Method
logp	3.073		Crippen Method
mcvol	157.470	ml/mol	McGowan Method
pc	2778.85	kPa	Joback Method
rinpol	1528.00		NIST Webbook
rinpol	1564.00		NIST Webbook
rinpol	1536.00		NIST Webbook
rinpol	1533.00		NIST Webbook
rinpol	1519.00		NIST Webbook
rinpol	1521.00		NIST Webbook
rinpol	1530.00		NIST Webbook
ripol	2158.00		NIST Webbook
ripol	2147.00		NIST Webbook
ripol	2174.00		NIST Webbook
ripol	2172.00		NIST Webbook
ripol	2152.00		NIST Webbook
ripol	2133.00		NIST Webbook
tb	600.62	K	Joback Method
tc	824.35	K	Joback Method
tf	349.67	K	Joback Method
vc	0.597	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	352.29	J/mol×K	600.62	Joback Method
cpg	364.97	J/mol×K	637.91	Joback Method
cpg	376.83	J/mol×K	675.20	Joback Method
cpg	387.90	J/mol×K	712.49	Joback Method
cpg	398.21	J/mol×K	749.77	Joback Method
cpg	407.80	J/mol×K	787.06	Joback Method
cpg	416.70	J/mol×K	824.35	Joback Method
dvisc	0.0014831	Pa×s	349.67	Joback Method
dvisc	0.0008442	Pa×s	391.50	Joback Method
dvisc	0.0005358	Pa×s	433.32	Joback Method
dvisc	0.0003684	Pa×s	475.14	Joback Method
dvisc	0.0002691	Pa×s	516.97	Joback Method
dvisc	0.0002060	Pa×s	558.79	Joback Method
dvisc	0.0001637	Pa×s	600.62	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=U373543&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