Prop-2-ynyl 3-chlorobenzoate

Other names: Benzoic acid, 3-chloro, 2-propynyl ester
Inchi: InChI=1S/C10H7ClO2/c1-2-6-13-10(12)8-4-3-5-9(11)7-8/h1,3-5,7H,6H2
InchiKey: LTRKIUGMBLDIDV-UHFFFAOYSA-N
Formula: C10H7ClO2
SMILES: C#CCOC(=O)c1cccc(Cl)c1
Mol. weight [g/mol]: 194.61

Physical Properties

Property code	Value	Unit	Source
gf	113.32	kJ/mol	Joback Method
hf	6.69	kJ/mol	Joback Method
hfus	25.27	kJ/mol	Joback Method
hvap	54.19	kJ/mol	Joback Method
log10ws	-3.03		Crippen Method
logp	2.130		Crippen Method
mcvol	139.080	ml/mol	McGowan Method
pc	3439.94	kPa	Joback Method
rinpol	1411.00		NIST Webbook
rinpol	1449.00		NIST Webbook
rinpol	1411.00		NIST Webbook
rinpol	1404.00		NIST Webbook
rinpol	1401.00		NIST Webbook
rinpol	1404.00		NIST Webbook
rinpol	1449.00		NIST Webbook
rinpol	1420.00		NIST Webbook
rinpol	1408.00		NIST Webbook
ripol	2194.00		NIST Webbook
ripol	2214.00		NIST Webbook
ripol	2208.00		NIST Webbook
ripol	2231.00		NIST Webbook
ripol	2222.00		NIST Webbook
ripol	2207.00		NIST Webbook
ripol	2194.00		NIST Webbook
ripol	2231.00		NIST Webbook
tb	563.70	K	Joback Method
tc	797.93	K	Joback Method
tf	390.45	K	Joback Method

vc	0.522	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	287.86	J/mol×K	563.70	Joback Method
cpg	298.70	J/mol×K	602.74	Joback Method
cpg	308.81	J/mol×K	641.78	Joback Method
cpg	318.22	J/mol×K	680.82	Joback Method
cpg	326.94	J/mol×K	719.86	Joback Method
cpg	335.00	J/mol×K	758.89	Joback Method
cpg	342.43	J/mol×K	797.93	Joback Method

Sources

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=U373549&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
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