

2-Chlorobenzoic acid, propargyl ester

Other names:	Benzoic acid, 2-chloro, 2-propynyl ester
Inchi:	InChI=1S/C10H7ClO2/c1-2-7-13-10(12)8-5-3-4-6-9(8)11/h1,3-6H,7H2
InchiKey:	KPSJNVKFAPXVOC-UHFFFAOYSA-N
Formula:	C10H7ClO2
SMILES:	C#CCOC(=O)c1ccccc1Cl
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	1429.00		NIST Webbook
rinpol	1410.00		NIST Webbook
rinpol	1414.00		NIST Webbook
rinpol	1409.00		NIST Webbook
rinpol	1410.00		NIST Webbook
rinpol	1422.00		NIST Webbook
rinpol	1420.00		NIST Webbook
ripol	2283.00		NIST Webbook
ripol	2310.00		NIST Webbook
ripol	2302.00		NIST Webbook
ripol	2331.00		NIST Webbook
ripol	2313.00		NIST Webbook
ripol	2298.00		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

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U325546&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
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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