Benzoic acid, 4-chloro, 2-propynyl ester

Inchi: InChI=1S/C10H7ClO2/c1-2-7-13-10(12)8-3-5-9(11)6-4-8/h1,3-6H,7H2
InchiKey: ZPVCGAZGDLPYDO-UHFFFAOYSA-N
Formula: C10H7ClO2
SMILES: C#CCOC(=O)c1ccc(Cl)cc1
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	1402.00		NIST Webbook
rinpol	1410.00		NIST Webbook
rinpol	1400.00		NIST Webbook
rinpol	1405.00		NIST Webbook
rinpol	1402.00		NIST Webbook
rinpol	1408.00		NIST Webbook
rinpol	1418.00		NIST Webbook
rinpol	1408.00		NIST Webbook
ripol	2190.00		NIST Webbook
ripol	2203.00		NIST Webbook
ripol	2231.00		NIST Webbook
ripol	2190.00		NIST Webbook
ripol	2204.00		NIST Webbook
ripol	2217.00		NIST Webbook
ripol	2231.00		NIST Webbook
ripol	2207.00		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

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=R31159&Units=SI

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