2-Chlorobenzoic acid, tridec-2-ynyl ester

Inchi: InChI=1S/C20H27ClO2/c1-2-3-4-5-6-7-8-9-10-11-14-17-23-20(22)18-15-12-13-16-19(18)
InchiKey: RDJRHBFOTCUIHH-UHFFFAOYSA-N
Formula: C20H27ClO2
SMILES: CCCCCCCCCCC#CCOC(=O)c1ccccc1Cl
Mol. weight [g/mol]: 334.88

Physical Properties

Property code	Value	Unit	Source
gf	177.25	kJ/mol	Joback Method
hf	-219.31	kJ/mol	Joback Method
hfus	51.31	kJ/mol	Joback Method
hvap	78.75	kJ/mol	Joback Method
log10ws	-7.22		Crippen Method
logp	6.031		Crippen Method
mcvol	279.980	ml/mol	McGowan Method
pc	1420.78	kPa	Joback Method
rinpol	2434.00		NIST Webbook
tb	811.38	K	Joback Method
tc	1021.00	K	Joback Method
tf	562.28	K	Joback Method
vc	1.083	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	807.37	J/mol×K	811.38	Joback Method
cpg	823.88	J/mol×K	846.32	Joback Method
cpg	839.32	J/mol×K	881.25	Joback Method
cpg	853.72	J/mol×K	916.19	Joback Method
cpg	867.12	J/mol×K	951.12	Joback Method
cpg	879.55	J/mol×K	986.06	Joback Method
cpg	891.06	J/mol×K	1021.00	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=U299306&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume