2-Chlorobenzoic acid, dodec-9-ynyl ester

Inchi: InChI=1S/C19H25ClO2/c1-2-3-4-5-6-7-8-9-10-13-16-22-19(21)17-14-11-12-15-18(17)20/
InchiKey: SUDQXLLPAJDXDC-UHFFFAOYSA-N
Formula: C19H25ClO2
SMILES: CCC#CCCCCCCCCOC(=O)c1ccccc1Cl
Mol. weight [g/mol]: 320.85

Physical Properties

Property code	Value	Unit	Source
gf	168.83	kJ/mol	Joback Method
hf	-198.67	kJ/mol	Joback Method
hfus	48.72	kJ/mol	Joback Method
hvap	76.52	kJ/mol	Joback Method
log10ws	-6.80		Crippen Method
logp	5.641		Crippen Method
mcvol	265.890	ml/mol	McGowan Method
pc	1529.46	kPa	Joback Method
rinpol	2343.90		NIST Webbook
rinpol	2343.90		NIST Webbook
tb	788.50	K	Joback Method
tc	999.73	K	Joback Method
tf	551.01	K	Joback Method
vc	1.026	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	749.93	J/mol×K	788.50	Joback Method
cpg	766.23	J/mol×K	823.70	Joback Method
cpg	781.48	J/mol×K	858.91	Joback Method
cpg	795.69	J/mol×K	894.11	Joback Method
cpg	808.92	J/mol×K	929.32	Joback Method
cpg	821.21	J/mol×K	964.52	Joback Method
cpg	832.57	J/mol×K	999.73	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=U292281&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