4-Chlorobenzoic acid, undec-2-enyl ester

Inchi: InChI=1S/C18H25ClO2/c1-2-3-4-5-6-7-8-9-10-15-21-18(20)16-11-13-17(19)14-12-16/h9-
InchiKey: OECIAGVCGLHDIB-MDZDMXLPSA-N
Formula: C18H25ClO2
SMILES: CCCCCCCCC=CCOC(=O)c1ccc(Cl)cc1
Mol. weight [g/mol]: 308.84

Physical Properties

Property code	Value	Unit	Source
gf	37.83	kJ/mol	Joback Method
hf	-333.11	kJ/mol	Joback Method
hfus	43.21	kJ/mol	Joback Method
hvap	72.10	kJ/mol	Joback Method
log10ws	-6.44		Crippen Method
logp	5.804		Crippen Method
mcvol	256.100	ml/mol	McGowan Method
pc	1515.21	kPa	Joback Method
rinpol	2241.00		NIST Webbook
tb	760.78	K	Joback Method
tc	963.40	K	Joback Method
tf	428.56	K	Joback Method
vc	0.989	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	716.95	J/mol×K	760.78	Joback Method
cpg	733.04	J/mol×K	794.55	Joback Method
cpg	748.15	J/mol×K	828.32	Joback Method
cpg	762.34	J/mol×K	862.09	Joback Method
cpg	775.65	J/mol×K	895.86	Joback Method
cpg	788.12	J/mol×K	929.63	Joback Method
cpg	799.79	J/mol×K	963.40	Joback Method
dvisc	0.0009520	Pa×s	428.56	Joback Method
dvisc	0.0004880	Pa×s	483.93	Joback Method

dvisc	0.0002869	Pa×s	539.30	Joback Method
dvisc	0.0001862	Pa×s	594.67	Joback Method
dvisc	0.0001301	Pa×s	650.04	Joback Method
dvisc	0.0000962	Pa×s	705.41	Joback Method
dvisc	0.0000743	Pa×s	760.78	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=U299370&Units=SI

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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

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