

2-Chlorobenzoic acid, tridecyl ester

Inchi:	InChI=1S/C20H31ClO2/c1-2-3-4-5-6-7-8-9-10-11-14-17-23-20(22)18-15-12-13-16-19(18)
InchiKey:	RIBWAZGMFLYEHT-UHFFFAOYSA-N
Formula:	C20H31ClO2
SMILES:	CCCCCCCCCCCCOC(=O)c1ccccc1Cl
Mol. weight [g/mol]:	338.91

Physical Properties

Property code	Value	Unit	Source
gf	-25.55	kJ/mol	Joback Method
hf	-491.61	kJ/mol	Joback Method
hfus	48.19	kJ/mol	Joback Method
hvap	76.59	kJ/mol	Joback Method
log10ws	-7.42		Crippen Method
logp	6.808		Crippen Method
mvol	288.580	ml/mol	McGowan Method
pc	1263.75	kPa	Joback Method
rinpol	2489.80		NIST Webbook
rinpol	2489.80		NIST Webbook
tb	802.38	K	Joback Method
tc	998.48	K	Joback Method
tf	456.18	K	Joback Method
vc	1.121	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	857.11	J/molxK	802.38	Joback Method
cpg	874.21	J/molxK	835.06	Joback Method
cpg	890.26	J/molxK	867.75	Joback Method
cpg	905.32	J/molxK	900.43	Joback Method
cpg	919.41	J/molxK	933.11	Joback Method
cpg	932.56	J/molxK	965.79	Joback Method
cpg	944.82	J/molxK	998.48	Joback Method
dvisc	0.0008547	Paxs	456.18	Joback Method

dvisc	0.0004381	Paxs	513.88	Joback Method
dvisc	0.0002570	Paxs	571.58	Joback Method
dvisc	0.0001662	Paxs	629.28	Joback Method
dvisc	0.0001157	Paxs	686.98	Joback Method
dvisc	0.0000852	Paxs	744.68	Joback Method
dvisc	0.0000655	Paxs	802.38	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U292428&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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