

2-Chlorobenzoic acid, 4-tridecyl ester

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

Physical Properties

Property code	Value	Unit	Source
gf	-27.99	kJ/mol	Joback Method
hf	-496.89	kJ/mol	Joback Method
hfus	44.67	kJ/mol	Joback Method
hvap	76.20	kJ/mol	Joback Method
log10ws	-7.53		Crippen Method
logp	6.806		Crippen Method
mvol	288.580	ml/mol	McGowan Method
pc	1270.97	kPa	Joback Method
rinpol	2286.00		NIST Webbook
rinpol	2286.00		NIST Webbook
tb	801.94	K	Joback Method
tc	1000.08	K	Joback Method
tf	441.18	K	Joback Method
vc	1.115	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	857.62	J/molxK	801.94	Joback Method
cpg	874.89	J/molxK	834.96	Joback Method
cpg	891.10	J/molxK	867.99	Joback Method
cpg	906.27	J/molxK	901.01	Joback Method
cpg	920.44	J/molxK	934.04	Joback Method
cpg	933.65	J/molxK	967.06	Joback Method
cpg	945.94	J/molxK	1000.08	Joback Method
dvisc	0.0009971	Paxs	441.18	Joback Method

dvisc	0.0004717	Paxs	501.31	Joback Method
dvisc	0.0002620	Paxs	561.43	Joback Method
dvisc	0.0001630	Paxs	621.56	Joback Method
dvisc	0.0001103	Paxs	681.69	Joback Method
dvisc	0.0000795	Paxs	741.81	Joback Method
dvisc	0.0000602	Paxs	801.94	Joback Method

Sources

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=U299816&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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