

4-Chlorobenzoic acid, dodecyl ester

Other names:	Dodecyl 4-chlorobenzoate
Inchi:	InChI=1S/C19H29ClO2/c1-2-3-4-5-6-7-8-9-10-11-16-22-19(21)17-12-14-18(20)15-13-17
InchiKey:	AEOLFEGHEDCXAW-UHFFFAOYSA-N
Formula:	C19H29ClO2
SMILES:	CCCCCCCCCCCCOC(=O)c1ccc(Cl)cc1
Mol. weight [g/mol]:	324.88
CAS:	97222-07-6

Physical Properties

Property code	Value	Unit	Source
gf	-33.97	kJ/mol	Joback Method
hf	-470.97	kJ/mol	Joback Method
hfus	45.60	kJ/mol	Joback Method
hvap	74.37	kJ/mol	Joback Method
log10ws	-7.00		Crippen Method
logp	6.418		Crippen Method
mcvol	274.490	ml/mol	McGowan Method
pc	1354.63	kPa	Joback Method
ripol	2322.00		NIST Webbook
ripol	2333.00		NIST Webbook
ripol	2363.00		NIST Webbook
ripol	2339.00		NIST Webbook
ripol	2351.00		NIST Webbook
ripol	2363.00		NIST Webbook
ripol	2312.00		NIST Webbook
ripol	2856.00		NIST Webbook
ripol	2856.00		NIST Webbook
ripol	2902.00		NIST Webbook
ripol	2880.00		NIST Webbook
ripol	2914.00		NIST Webbook
ripol	2898.00		NIST Webbook
ripol	2874.00		NIST Webbook
tb	779.50	K	Joback Method
tc	975.71	K	Joback Method
tf	444.91	K	Joback Method
vc	1.065	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	798.77	J/molxK	779.50	Joback Method
cpg	873.21	J/molxK	943.01	Joback Method
cpg	860.21	J/molxK	910.31	Joback Method
cpg	846.30	J/molxK	877.61	Joback Method
cpg	831.45	J/molxK	844.90	Joback Method
cpg	815.62	J/molxK	812.20	Joback Method
cpg	885.33	J/molxK	975.71	Joback Method
dvisc	0.0000750	Paxs	779.50	Joback Method
dvisc	0.0000972	Paxs	723.73	Joback Method
dvisc	0.0001315	Paxs	667.97	Joback Method
dvisc	0.0001880	Paxs	612.20	Joback Method
dvisc	0.0002888	Paxs	556.44	Joback Method
dvisc	0.0004880	Paxs	500.68	Joback Method
dvisc	0.0009407	Paxs	444.91	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C97222076&Units=SI
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

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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