

2-Chlorobenzoic acid, 4-tetradecyl ester

Inchi:	InChI=1S/C21H33ClO2/c1-3-5-6-7-8-9-10-11-15-18(14-4-2)24-21(23)19-16-12-13-17-20
InchiKey:	YCRAQMYJTQYHQF-UHFFFAOYSA-N
Formula:	C21H33ClO2
SMILES:	CCCCCCCCCCC(CCC)OC(=O)c1ccccc1Cl
Mol. weight [g/mol]:	352.94

Physical Properties

Property code	Value	Unit	Source
gf	-19.57	kJ/mol	Joback Method
hf	-517.53	kJ/mol	Joback Method
hfus	47.26	kJ/mol	Joback Method
hvap	78.43	kJ/mol	Joback Method
log10ws	-7.95		Crippen Method
logp	7.196		Crippen Method
mvol	302.670	ml/mol	McGowan Method
pc	1188.24	kPa	Joback Method
rinpol	2390.00		NIST Webbook
rinpol	2390.00		NIST Webbook
tb	824.82	K	Joback Method
tc	1023.18	K	Joback Method
tf	452.45	K	Joback Method
vc	1.171	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	916.82	J/molxK	824.82	Joback Method
cpg	934.32	J/molxK	857.88	Joback Method
cpg	950.71	J/molxK	890.94	Joback Method
cpg	966.05	J/molxK	924.00	Joback Method
cpg	980.36	J/molxK	957.06	Joback Method
cpg	993.70	J/molxK	990.12	Joback Method
cpg	1006.09	J/molxK	1023.18	Joback Method
dvisc	0.0008970	Paxs	452.45	Joback Method

dvisc	0.0004199	Paxs	514.51	Joback Method
dvisc	0.0002314	Paxs	576.57	Joback Method
dvisc	0.0001432	Paxs	638.63	Joback Method
dvisc	0.0000965	Paxs	700.70	Joback Method
dvisc	0.0000693	Paxs	762.76	Joback Method
dvisc	0.0000523	Paxs	824.82	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=U299819&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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