

2-Chlorobenzoic acid, 4-hexadecyl ester

Inchi:	InChI=1S/C23H37ClO2/c1-3-5-6-7-8-9-10-11-12-13-17-20(16-4-2)26-23(25)21-18-14-15
InchiKey:	RLHBBBCVZFMPQH-UHFFFAOYSA-N
Formula:	C23H37ClO2
SMILES:	CCCCCCCCCCCC(CCC)OC(=O)c1ccccc1Cl
Mol. weight [g/mol]:	380.99

Physical Properties

Property code	Value	Unit	Source
gf	-2.73	kJ/mol	Joback Method
hf	-558.81	kJ/mol	Joback Method
hfus	52.44	kJ/mol	Joback Method
hvap	82.88	kJ/mol	Joback Method
log10ws	-8.79		Crippen Method
logp	7.977		Crippen Method
mvol	330.850	ml/mol	McGowan Method
pc	1045.30	kPa	Joback Method
rinpol	2479.10		NIST Webbook
rinpol	2479.10		NIST Webbook
tb	870.58	K	Joback Method
tc	1071.46	K	Joback Method
tf	474.99	K	Joback Method
vc	1.282	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1037.58	J/molxK	870.58	Joback Method
cpg	1116.14	J/molxK	1037.98	Joback Method
cpg	1102.58	J/molxK	1004.50	Joback Method
cpg	1087.99	J/molxK	971.02	Joback Method
cpg	1072.33	J/molxK	937.54	Joback Method
cpg	1055.54	J/molxK	904.06	Joback Method
cpg	1128.72	J/molxK	1071.46	Joback Method
dvisc	0.0000393	Paxs	870.58	Joback Method

dvisc	0.0000523	Paxs	804.65	Joback Method
dvisc	0.0000732	Paxs	738.72	Joback Method
dvisc	0.0001096	Paxs	672.78	Joback Method
dvisc	0.0001789	Paxs	606.85	Joback Method
dvisc	0.0003291	Paxs	540.92	Joback Method
dvisc	0.0007172	Paxs	474.99	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=U292282&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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