

4-Chlorobenzoic acid, 2-naphthyl ester

Inchi:	InChI=1S/C17H11ClO2/c18-15-8-5-13(6-9-15)17(19)20-16-10-7-12-3-1-2-4-14(12)11-16
InchiKey:	HFTVSEPAGVIKQA-UHFFFAOYSA-N
Formula:	C17H11ClO2
SMILES:	O=C(Oc1ccc2ccccc2c1)c1ccc(Cl)cc1
Mol. weight [g/mol]:	282.72

Physical Properties

Property code	Value	Unit	Source
gf	158.62	kJ/mol	Joback Method
hf	-13.56	kJ/mol	Joback Method
hfus	31.09	kJ/mol	Joback Method
hvap	74.49	kJ/mol	Joback Method
log10ws	-6.05		Crippen Method
logp	4.712		Crippen Method
mcvol	203.090	ml/mol	McGowan Method
pc	2592.49	kPa	Joback Method
rinpol	2424.00		NIST Webbook
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tb	784.38	K	Joback Method
tc	1043.72	K	Joback Method
tf	494.01	K	Joback Method
vc	0.766	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	524.43	J/molxK	784.38	Joback Method
cpg	537.35	J/molxK	827.60	Joback Method
cpg	549.09	J/molxK	870.83	Joback Method
cpg	559.77	J/molxK	914.05	Joback Method
cpg	569.49	J/molxK	957.27	Joback Method
cpg	578.35	J/molxK	1000.49	Joback Method
cpg	586.46	J/molxK	1043.72	Joback Method
dvisc	0.0009274	Paxs	494.01	Joback Method

dvisc	0.0006327	Paxs	542.41	Joback Method
dvisc	0.0004595	Paxs	590.80	Joback Method
dvisc	0.0003503	Paxs	639.20	Joback Method
dvisc	0.0002774	Paxs	687.59	Joback Method
dvisc	0.0002266	Paxs	735.99	Joback Method
dvisc	0.0001897	Paxs	784.38	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=U307763&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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