

2-Chlorobenzoic acid, cyclobutyl ester

Inchi:	InChI=1S/C11H11ClO2/c12-10-7-2-1-6-9(10)11(13)14-8-4-3-5-8/h1-2,6-8H,3-5H2
InchiKey:	CDMUMZPSCNDTJY-UHFFFAOYSA-N
Formula:	C11H11ClO2
SMILES:	O=C(OC1CCC1)c1ccccc1Cl
Mol. weight [g/mol]:	210.66

Physical Properties

Property code	Value	Unit	Source
gf	-52.68	kJ/mol	Joback Method
hf	-239.21	kJ/mol	Joback Method
hfus	20.92	kJ/mol	Joback Method
hvap	56.64	kJ/mol	Joback Method
log10ws	-3.66		Crippen Method
logp	3.049		Crippen Method
mcvol	150.910	ml/mol	McGowan Method
pc	3107.10	kPa	Joback Method
rinpola	1586.60		NIST Webbook
tb	607.47	K	Joback Method
tc	845.52	K	Joback Method
tf	369.17	K	Joback Method
vc	0.566	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	358.89	J/molxK	607.47	Joback Method
cpg	373.56	J/molxK	647.14	Joback Method
cpg	387.15	J/molxK	686.82	Joback Method
cpg	399.72	J/molxK	726.49	Joback Method
cpg	411.32	J/molxK	766.17	Joback Method
cpg	421.99	J/molxK	805.84	Joback Method
cpg	431.79	J/molxK	845.52	Joback Method
dvisc	0.0018581	Paxs	369.17	Joback Method
dvisc	0.0012308	Paxs	408.89	Joback Method

dvisc	0.0008770	Paxs	448.60	Joback Method
dvisc	0.0006603	Paxs	488.32	Joback Method
dvisc	0.0005188	Paxs	528.04	Joback Method
dvisc	0.0004216	Paxs	567.75	Joback Method
dvisc	0.0003521	Paxs	607.47	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U292275&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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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