

3-Oxobutan-2-yl 3-chlorobenzoate

Inchi:	InChI=1S/C11H11ClO3/c1-7(13)8(2)15-11(14)9-4-3-5-10(12)6-9/h3-6,8H,1-2H3
InchiKey:	YXSJHBJFQZIWCD-UHFFFAOYSA-N
Formula:	C11H11ClO3
SMILES:	CC(=O)C(C)OC(=O)c1cccc(Cl)c1
Mol. weight [g/mol]:	226.66

Physical Properties

Property code	Value	Unit	Source
gf	-232.69	kJ/mol	Joback Method
hf	-423.71	kJ/mol	Joback Method
hfus	22.96	kJ/mol	Joback Method
hvap	62.92	kJ/mol	Joback Method
log10ws	-3.05		Crippen Method
logp	2.474		Crippen Method
mcvol	163.340	ml/mol	McGowan Method
pc	2835.36	kPa	Joback Method
rinpola	1617.00		NIST Webbook
tb	649.89	K	Joback Method
tc	875.66	K	Joback Method
tf	389.68	K	Joback Method
vc	0.617	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	387.69	J/molxK	649.89	Joback Method
cpg	399.94	J/molxK	687.52	Joback Method
cpg	411.33	J/molxK	725.15	Joback Method
cpg	421.90	J/molxK	762.78	Joback Method
cpg	431.66	J/molxK	800.41	Joback Method
cpg	440.63	J/molxK	838.04	Joback Method
cpg	448.82	J/molxK	875.66	Joback Method
dvisc	0.0016763	Paxs	389.68	Joback Method
dvisc	0.0009642	Paxs	433.05	Joback Method

dvisc	0.0006134	Paxs	476.42	Joback Method
dvisc	0.0004208	Paxs	519.78	Joback Method
dvisc	0.0003059	Paxs	563.15	Joback Method
dvisc	0.0002328	Paxs	606.52	Joback Method
dvisc	0.0001837	Paxs	649.89	Joback Method

Sources

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=U373544&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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