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
hf	-329.12	kJ/mol	Cheméo Relay (1.0)
hfus	20.92	kJ/mol	Joback Method
ie	9.13	eV	Cheméo Relay (1.0)
log10ws	-3.70		Cheméo Relay (1.0)
logp	3.049		Crippen Method
mcvol	150.910	ml/mol	McGowan Method
rinpol	1586.60		NIST Webbook
tb	556.79	K	Cheméo Relay (1.0)
tf	245.66	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	358.89	J/mol×K	607.47	Joback Method
cpg	431.79	J/mol×K	845.52	Joback Method
cpg	421.99	J/mol×K	805.84	Joback Method
cpg	411.32	J/mol×K	766.17	Joback Method
cpg	399.72	J/mol×K	726.49	Joback Method
cpg	387.15	J/mol×K	686.82	Joback Method
cpg	373.56	J/mol×K	647.14	Joback Method
dvisc	0.0006603	Pa×s	488.32	Joback Method
dvisc	0.0003521	Pa×s	607.47	Joback Method
dvisc	0.0004216	Pa×s	567.75	Joback Method
dvisc	0.0005188	Pa×s	528.04	Joback Method
dvisc	0.0018581	Pa×s	369.17	Joback Method
dvisc	0.0008770	Pa×s	448.60	Joback Method

dvisc	0.0012308	Pa×s	408.89	Joback Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U292275&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
ie: Ionization energy
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tf: Normal melting (fusion) point