2,3-Difluorobenzoylchloride

Inchi: InChI=1S/C7H3ClF2O/c8-7(11)4-2-1-3-5(9)6(4)10/h1-3H
InchiKey: CDCFERWURRNLLA-UHFFFAOYSA-N
Formula: C7H3ClF2O
SMILES: O=C(Cl)c1cccc(F)c1F
Mol. weight [g/mol]: 176.55

Physical Properties

Property code	Value	Unit	Source
hfus	19.11	kJ/mol	Joback Method
ie	9.80	eV	Cheméo Relay (1.0)
logp	2.344		Crippen Method
mcvol	103.080	ml/mol	McGowan Method
tb	454.11	K	Cheméo Relay (1.0)
tf	251.72	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	192.28	J/mol×K	486.04	Joback Method
cpg	200.24	J/mol×K	521.04	Joback Method
cpg	207.73	J/mol×K	556.05	Joback Method
cpg	214.74	J/mol×K	591.05	Joback Method
cpg	221.31	J/mol×K	626.06	Joback Method
cpg	227.44	J/mol×K	661.06	Joback Method
cpg	233.14	J/mol×K	696.07	Joback Method

Sources

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):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C18355732&Units=SI

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

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point