2,3-DIFLUOROBENZOIC ACID

Inchi: InChI=1S/C7H4F2O2/c8-5-3-1-2-4(6(5)9)7(10)11/h1-3H,(H,10,11)
InchiKey: JLZVIWSFUPLSOR-UHFFFAOYSA-N
Formula: C7H4F2O2
SMILES: O=C(O)c1cccc(F)c1F
Mol. weight [g/mol]: 158.10

Physical Properties

Property code	Value	Unit	Source
hf	-662.44	kJ/mol	Cheméo Relay (1.0)
hfus	19.00	kJ/mol	Joback Method
ie	9.64	eV	Cheméo Relay (1.0)
log10ws	-2.02		Cheméo Relay (1.0)
logp	1.663		Crippen Method
mcvol	96.710	ml/mol	McGowan Method
tb	498.52	K	Cheméo Relay (1.0)
tc	723.80	K	Cheméo Relay (1.0)
tf	388.92	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	208.83	J/mol×K	540.79	Joback Method
cpg	215.99	J/mol×K	572.79	Joback Method
cpg	222.74	J/mol×K	604.78	Joback Method
cpg	229.10	J/mol×K	636.78	Joback Method
cpg	235.09	J/mol×K	668.77	Joback Method
cpg	240.70	J/mol×K	700.77	Joback Method
cpg	245.97	J/mol×K	732.76	Joback Method

Sources

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):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4519395&Units=SI

Legend

cpg:	Ideal gas heat capacity
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point