4-Fluoro-2-(trifluoromethyl)benzaldehyde

Inchi: InChI=1S/C8H4F4O/c9-6-2-1-5(4-13)7(3-6)8(10,11)12/h1-4H
InchiKey: NONOHEMDNFTKCZ-UHFFFAOYSA-N
Formula: C8H4F4O
SMILES: O=Cc1ccc(F)cc1C(F)(F)F
Mol. weight [g/mol]: 192.11
CAS: 90176-80-0

Physical Properties

Property code	Value	Unit	Source
gf	-766.29	kJ/mol	Joback Method
hf	-873.63	kJ/mol	Joback Method
hfus	16.93	kJ/mol	Joback Method
hvap	39.16	kJ/mol	Joback Method
log10ws	-3.15		Crippen Method
logp	2.657		Crippen Method
mcvol	108.470	ml/mol	McGowan Method
pc	3184.73	kPa	Joback Method
tb	461.59	K	Joback Method
tc	649.64	K	Joback Method
tf	278.16	K	Joback Method
vc	0.454	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	231.01	J/mol×K	461.59	Joback Method
cpg	240.50	J/mol×K	492.93	Joback Method
cpg	249.38	J/mol×K	524.27	Joback Method
cpg	257.66	J/mol×K	555.62	Joback Method
cpg	265.38	J/mol×K	586.96	Joback Method
cpg	272.57	J/mol×K	618.30	Joback Method
cpg	279.26	J/mol×K	649.64	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C90176800&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

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