2-Fluorobenzyl trifluoroacetate

Inchi: InChI=1S/C9H6F4O2/c10-7-4-2-1-3-6(7)5-15-8(14)9(11,12)13/h1-4H,5H2
InchiKey: LSTCWVISNNEWAM-UHFFFAOYSA-N
Formula: C9H6F4O2
SMILES: O=C(OCc1ccccc1F)C(F)(F)F
Mol. weight [g/mol]: 222.14

Physical Properties

Property code	Value	Unit	Source
gf	-882.64	kJ/mol	Joback Method
hf	-1042.02	kJ/mol	Joback Method
hfus	20.41	kJ/mol	Joback Method
hvap	43.16	kJ/mol	Joback Method
log10ws	-3.04		Crippen Method
logp	2.431		Crippen Method
mcvol	128.430	ml/mol	McGowan Method
pc	2826.33	kPa	Joback Method
rinpol	1003.00		NIST Webbook
rinpol	1003.00		NIST Webbook
tb	507.12	K	Joback Method
tc	695.63	K	Joback Method
tf	307.07	K	Joback Method
vc	0.516	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	292.95	J/mol×K	507.12	Joback Method
cpg	303.76	J/mol×K	538.54	Joback Method
cpg	313.92	J/mol×K	569.96	Joback Method
cpg	323.44	J/mol×K	601.37	Joback Method
cpg	332.35	J/mol×K	632.79	Joback Method
cpg	340.68	J/mol×K	664.21	Joback Method
cpg	348.45	J/mol×K	695.63	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=U373474&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
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