2-Fluoro-6-(trifluoromethyl)benzyl alcohol

Inchi: InChI=1S/C8H6F4O/c9-7-3-1-2-6(5(7)4-13)8(10,11)12/h1-3,13H,4H2
InchiKey: TZUCYZIRXZYZOP-UHFFFAOYSA-N
Formula: C8H6F4O
SMILES: OCc1c(F)cccc1C(F)(F)F
Mol. weight [g/mol]: 194.13
CAS: 152211-15-9

Physical Properties

Property code	Value	Unit	Source
gf	-803.59	kJ/mol	Joback Method
hf	-940.28	kJ/mol	Joback Method
hfus	18.73	kJ/mol	Joback Method
hvap	49.12	kJ/mol	Joback Method
log10ws	-3.05		Crippen Method
logp	2.337		Crippen Method
mcvol	112.770	ml/mol	McGowan Method
pc	3250.43	kPa	Joback Method
tb	505.11	K	Joback Method
tc	679.44	K	Joback Method
tf	296.98	K	Joback Method
vc	0.456	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	259.96	J/mol×K	505.11	Joback Method
cpg	268.87	J/mol×K	534.17	Joback Method
cpg	277.25	J/mol×K	563.22	Joback Method
cpg	285.13	J/mol×K	592.28	Joback Method
cpg	292.52	J/mol×K	621.33	Joback Method
cpg	299.45	J/mol×K	650.39	Joback Method
cpg	305.96	J/mol×K	679.44	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C152211159&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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