2-Fluoro-.alpha.-methylbenzyl alcohol

Other names: o-Fluorophenylmethylcarbinol
Benzenemethanol, 2-fluoro-«alpha»-methyl-
2-fluoro-«alpha»-methylbenzyl alcohol
Inchi: InChI=1S/C8H9FO/c1-6(10)7-4-2-3-5-8(7)9/h2-6,10H,1H3
InchiKey: SXFYVXSOEBCFLV-UHFFFAOYSA-N
Formula: C8H9FO
SMILES: CC(O)c1ccccc1F
Mol. weight [g/mol]: 140.16

Physical Properties

Property code	Value	Unit	Source
hf	-374.69	kJ/mol	Cheméo Relay (1.0)
hfus	13.77	kJ/mol	Joback Method
hvap	71.97	kJ/mol	Cheméo Relay (1.0)
ie	9.12	eV	Cheméo Relay (1.0)
log10ws	-0.77		Cheméo Relay (1.0)
logp	1.879		Crippen Method
mcvol	107.460	ml/mol	McGowan Method
pc	3834.03	kPa	Joback Method
tb	454.47	K	Cheméo Relay (1.0)
tc	678.39	K	Cheméo Relay (1.0)
tf	306.52	K	Cheméo Relay (1.0)
vc	0.393	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	231.98	J/mol×K	505.11	Joback Method
cpg	242.10	J/mol×K	537.28	Joback Method
cpg	251.67	J/mol×K	569.44	Joback Method
cpg	260.71	J/mol×K	601.61	Joback Method
cpg	269.25	J/mol×K	633.78	Joback Method
cpg	277.29	J/mol×K	665.95	Joback Method
cpg	284.87	J/mol×K	698.11	Joback Method

Sources

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=C445261&Units=SI
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
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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