Benzenemethanol, 3-fluoro-«alpha»-methyl-

Other names: 3-Fluorophenylmethylcarbinol
m-Fluorophenylmethylcarbinol
m-Fluoro-«alpha»-methylbenzyl alcohol
3-fluoro-«alpha»-methylbenzyl alcohol
Inchi: InChI=1S/C8H9FO/c1-6(10)7-3-2-4-8(9)5-7/h2-6,10H,1H3
InchiKey: YESOPGLEIJQAEF-UHFFFAOYSA-N
Formula: C8H9FO
SMILES: CC(O)c1cccc(F)c1
Mol. weight [g/mol]: 140.15
CAS: 402-63-1

Physical Properties

Property code	Value	Unit	Source
gf	-214.81	kJ/mol	Joback Method
hf	-337.01	kJ/mol	Joback Method
hfus	13.77	kJ/mol	Joback Method
hvap	51.81	kJ/mol	Joback Method
log10ws	-2.33		Crippen Method
logp	1.879		Crippen Method
mcvol	107.460	ml/mol	McGowan Method
pc	3834.03	kPa	Joback Method
rinpol	1048.60		NIST Webbook
tb	505.11	K	Joback Method
tc	698.11	K	Joback Method
tf	265.27	K	Joback Method
vc	0.406	m3/kmol	Joback Method

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

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C402631&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume