

Benzenemethanol, 3-fluoro-

Other names:	Benzyl alcohol, m-fluoro- m-Fluorobenzyl alcohol 3-Fluorobenzyl alcohol 3-fluorobenzyl alcohol
Inchi:	InChI=1S/C7H7FO/c8-7-3-1-2-6(4-7)5-9/h1-4,9H,5H2
InchiKey:	QDHRSLFSDGCJFX-UHFFFAOYSA-N
Formula:	C7H7FO
SMILES:	OCc1cccc(F)c1
Mol. weight [g/mol]:	126.13
CAS:	456-47-3

Physical Properties

Property code	Value	Unit	Source
gf	-220.79	kJ/mol	Joback Method
hf	-311.09	kJ/mol	Joback Method
hfus	14.71	kJ/mol	Joback Method
hvap	49.98	kJ/mol	Joback Method
log10ws	-1.95		Crippen Method
logp	1.318		Crippen Method
mcvol	93.370	ml/mol	McGowan Method
pc	4288.66	kPa	Joback Method
tb	377.50 ± 0.50	K	NIST Webbook
tc	673.82	K	Joback Method
tf	269.00	K	Joback Method
vc	0.356	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	190.60	J/mol×K	482.67	Joback Method
cpg	199.36	J/mol×K	514.53	Joback Method
cpg	207.65	J/mol×K	546.39	Joback Method
cpg	215.49	J/mol×K	578.25	Joback Method
cpg	222.89	J/mol×K	610.10	Joback Method

cpg	229.87	J/mol×K	641.96	Joback Method
cpg	236.44	J/mol×K	673.82	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	377.70	K	2.90	NIST Webbook

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C456473&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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