

O-FLUOROBENZYL ALCOHOL

Other names:	o-Fluorobenzyl alcohol Benzenemethanol, 2-fluoro- 2-fluorobenzyl alcohol
Inchi:	InChI=1S/C7H7FO/c8-7-4-2-1-3-6(7)5-9/h1-4,9H,5H2
InchiKey:	QEHXDOJPVIHUO-UHFFFAOYSA-N
Formula:	C7H7FO
SMILES:	OCc1ccccc1F
Mol. weight [g/mol]:	126.13

Physical Properties

Property code	Value	Unit	Source
hf	-320.98	kJ/mol	Cheméo Relay (1.0)
hfus	14.71	kJ/mol	Joback Method
hvap	70.38	kJ/mol	Cheméo Relay (1.0)
ie	8.99	eV	Cheméo Relay (1.0)
log10ws	-0.78		Cheméo Relay (1.0)
logp	1.318		Crippen Method
mcvol	93.370	ml/mol	McGowan Method
tb	472.50 ± 0.50	K	NIST Webbook
tc	698.72	K	Cheméo Relay (1.0)
tf	299.03	K	Cheméo Relay (1.0)

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

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C446515&Units=SI>

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

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):

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point

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