

4-Fluoro-o-cresol

Inchi:	InChI=1S/C7H7FO/c1-5-4-6(8)2-3-7(5)9/h2-4,9H,1H3
InchiKey:	GKQDDKKGDIVDAG-UHFFFAOYSA-N
Formula:	C7H7FO
SMILES:	Cc1cc(F)ccc1O
Mol. weight [g/mol]:	126.13
CAS:	452-72-2

Physical Properties

Property code	Value	Unit	Source
gf	-238.59	kJ/mol	Joback Method
hf	-336.17	kJ/mol	Joback Method
hfus	16.40	kJ/mol	Joback Method
hvap	46.31	kJ/mol	Joback Method
log10ws	-1.83		Crippen Method
logp	1.840		Crippen Method
mcvol	93.370	ml/mol	McGowan Method
pc	4627.70	kPa	Joback Method
tb	471.11	K	Joback Method
tc	689.77	K	Joback Method
tf	319.90	K	Joback Method
vc	0.303	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	192.66	J/mol×K	471.11	Joback Method
cpg	202.40	J/mol×K	507.55	Joback Method
cpg	211.43	J/mol×K	544.00	Joback Method
cpg	219.79	J/mol×K	580.44	Joback Method
cpg	227.56	J/mol×K	616.88	Joback Method
cpg	234.79	J/mol×K	653.33	Joback Method
cpg	241.54	J/mol×K	689.77	Joback Method

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=C452722&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
hvac:	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

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