

Ethanethiol, 2-(p-fluoroanilino)-

Inchi:	InChI=1S/C8H10FNS/c9-7-1-3-8(4-2-7)10-5-6-11/h1-4,10-11H,5-6H2
InchiKey:	XDVPEFZFQHGYYDA-UHFFFAOYSA-N
Formula:	C8H10FNS
SMILES:	Fc1ccc(NCCS)cc1
Mol. weight [g/mol]:	171.24
CAS:	20295-60-7

Physical Properties

Property code	Value	Unit	Source
gf	43.23	kJ/mol	Joback Method
hf	-87.55	kJ/mol	Joback Method
hfus	22.35	kJ/mol	Joback Method
hvap	48.70	kJ/mol	Joback Method
log10ws	-2.30		Crippen Method
logp	2.167		Crippen Method
mvol	127.920	ml/mol	McGowan Method
pc	3727.11	kPa	Joback Method
tb	526.40	K	Joback Method
tc	750.42	K	Joback Method
tf	308.57	K	Joback Method
vc	0.482	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	272.91	J/mol×K	526.40	Joback Method
cpg	285.26	J/mol×K	563.74	Joback Method
cpg	296.82	J/mol×K	601.07	Joback Method
cpg	307.62	J/mol×K	638.41	Joback Method
cpg	317.70	J/mol×K	675.74	Joback Method
cpg	327.10	J/mol×K	713.08	Joback Method
cpg	335.83	J/mol×K	750.42	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C20295607&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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

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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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