

Ethanol, 2-[(4-nitrophenyl)thio]-

Inchi:	InChI=1S/C8H9NO3S/c10-5-6-13-8-3-1-7(2-4-8)9(11)12/h1-4,10H,5-6H2
InchiKey:	RVYZERYSWJUJY-UHFFFAOYSA-N
Formula:	C8H9NO3S
SMILES:	O=[N+](O)c1ccc(SCCO)cc1
Mol. weight [g/mol]:	199.23
CAS:	13287-76-8

Physical Properties

Property code	Value	Unit	Source
gf	51.11	kJ/mol	Joback Method
hf	-104.51	kJ/mol	Joback Method
hfus	29.71	kJ/mol	Joback Method
hvap	76.43	kJ/mol	Joback Method
log10ws	-2.55		Crippen Method
logp	1.679		Crippen Method
mcvol	139.460	ml/mol	McGowan Method
pc	4167.71	kPa	Joback Method
tb	726.90	K	Joback Method
tc	965.99	K	Joback Method
tf	457.69	K	Joback Method
vc	0.530	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	352.43	J/molxK	726.90	Joback Method
cpg	361.78	J/molxK	766.75	Joback Method
cpg	370.36	J/molxK	806.60	Joback Method
cpg	378.18	J/molxK	846.44	Joback Method
cpg	385.30	J/molxK	886.29	Joback Method
cpg	391.74	J/molxK	926.14	Joback Method
cpg	397.53	J/molxK	965.99	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C13287768&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

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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