Aniline, 5-(methylsulfonyl)-2-propoxy-

Inchi: InChI=1S/C10H15NO3S/c1-3-6-14-10-5-4-8(7-9(10)11)15(2,12)13/h4-5,7H,3,6,11H2,1-2
InchiKey: ITXAUAOQDSMOQH-UHFFFAOYSA-N
Formula: C10H15NO3S
SMILES: CCCOc1ccc(S(C)(=O)=O)cc1N
Mol. weight [g/mol]: 229.30
CAS: 91252-74-3

Physical Properties

Property code	Value	Unit	Source
gf	-380.62	kJ/mol	Joback Method
hf	-587.92	kJ/mol	Joback Method
hfus	32.68	kJ/mol	Joback Method
hvap	73.14	kJ/mol	Joback Method
log10ws	-1.76		Crippen Method
logp	1.461		Crippen Method
mcvol	171.940	ml/mol	McGowan Method
pc	3534.66	kPa	Joback Method
tb	607.57	K	Joback Method
tc	815.20	K	Joback Method
tf	397.97	K	Joback Method
vc	0.660	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	422.48	J/mol×K	607.57	Joback Method
cpg	436.51	J/mol×K	642.17	Joback Method
cpg	449.76	J/mol×K	676.78	Joback Method
cpg	462.21	J/mol×K	711.38	Joback Method
cpg	473.86	J/mol×K	745.99	Joback Method
cpg	484.71	J/mol×K	780.59	Joback Method
cpg	494.74	J/mol×K	815.20	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C91252743&Units=SI

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