P-nitro ethane sulfoanilide

Inchi: InChI=1S/C8H10N2O4S/c1-2-15(13,14)9-7-3-5-8(6-4-7)10(11)12/h3-6,9H,2H2,1H3
InchiKey: ZENKIQMTPMONLY-UHFFFAOYSA-N
Formula: C8H10N2O4S
SMILES: CCS(=O)(=O)Nc1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]: 230.24
CAS: 57616-17-8

Physical Properties

Property code	Value	Unit	Source
gf	-224.34	kJ/mol	Joback Method
hf	-394.03	kJ/mol	Joback Method
hfus	37.97	kJ/mol	Joback Method
hvap	78.00	kJ/mol	Joback Method
log10ws	-2.37		Crippen Method
logp	1.356		Crippen Method
mcvol	155.310	ml/mol	McGowan Method
pc	4504.30	kPa	Joback Method
tb	663.89	K	Joback Method
tc	895.32	K	Joback Method
tf	453.69	K	Joback Method
vc	0.619	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	390.13	J/mol×K	663.89	Joback Method
cpg	402.09	J/mol×K	702.46	Joback Method
cpg	413.07	J/mol×K	741.03	Joback Method
cpg	423.09	J/mol×K	779.61	Joback Method
cpg	432.17	J/mol×K	818.18	Joback Method
cpg	440.32	J/mol×K	856.75	Joback Method
cpg	447.58	J/mol×K	895.32	Joback Method

Sources

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=C57616178&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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