P-toluenesulfonamide, n-(4-acetamidobutyl)-

Inchi: InChI=1S/C13H20N2O3S/c1-11-5-7-13(8-6-11)19(17,18)15-10-4-3-9-14-12(2)16/h5-8,15
InchiKey: QXVMZVAQQKTYMB-UHFFFAOYSA-N
Formula: C13H20N2O3S
SMILES: CC(=O)NCCCCNS(=O)(=O)c1ccc(C)cc1
Mol. weight [g/mol]: 284.38
CAS: 15440-82-1

Physical Properties

Property code	Value	Unit	Source
gf	-257.32	kJ/mol	Joback Method
hf	-545.58	kJ/mol	Joback Method
hfus	46.25	kJ/mol	Joback Method
hvap	85.72	kJ/mol	Joback Method
log10ws	-2.88		Crippen Method
logp	1.190		Crippen Method
mcvol	219.890	ml/mol	McGowan Method
pc	2752.67	kPa	Joback Method
tb	730.49	K	Joback Method
tc	931.18	K	Joback Method
tf	469.02	K	Joback Method
vc	0.858	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	612.68	J/mol×K	730.49	Joback Method
cpg	626.96	J/mol×K	763.94	Joback Method
cpg	640.24	J/mol×K	797.39	Joback Method
cpg	652.54	J/mol×K	830.83	Joback Method
cpg	663.88	J/mol×K	864.28	Joback Method
cpg	674.28	J/mol×K	897.73	Joback Method
cpg	683.76	J/mol×K	931.18	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C15440821&Units=SI
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

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