N-propylsulfonyl-2-propanone

Inchi: InChI=1S/C6H12O3S/c1-3-4-10(8,9)5-6(2)7/h3-5H2,1-2H3
InchiKey: GIBVRWNWIPWWSI-UHFFFAOYSA-N
Formula: C6H12O3S
SMILES: CCCS(=O)(=O)CC(C)=O
Mol. weight [g/mol]: 164.22
CAS: 91313-63-2

Physical Properties

Property code	Value	Unit	Source
gf	-597.82	kJ/mol	Joback Method
hf	-733.10	kJ/mol	Joback Method
hfus	24.27	kJ/mol	Joback Method
hvap	54.33	kJ/mol	Joback Method
log10ws	-0.45		Crippen Method
logp	0.400		Crippen Method
mcvol	125.060	ml/mol	McGowan Method
pc	4026.13	kPa	Joback Method
tb	438.33	K	Joback Method
tc	613.06	K	Joback Method
tf	245.87	K	Joback Method
vc	0.503	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	249.06	J/mol×K	438.33	Joback Method
cpg	259.96	J/mol×K	467.45	Joback Method
cpg	270.46	J/mol×K	496.57	Joback Method
cpg	280.56	J/mol×K	525.70	Joback Method
cpg	290.26	J/mol×K	554.82	Joback Method
cpg	299.55	J/mol×K	583.94	Joback Method
cpg	308.44	J/mol×K	613.06	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=C91313632&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