Isopropylsulfonyl chloride

Other names:	Propane-2-sulfonyl chloride
	2-Propanesulfonyl chloride
	isopropylsulphonyl chloride
Inchi:	InChI=1S/C3H7ClO2S/c1-3(2)7(4,5)6/h3H,1-2H3
InchiKey:	DRINJBFRTLBHNF-UHFFFAOYSA-N
Formula:	C3H7ClO2S
SMILES:	CC(C)S(=O)(=O)Cl
Mol. weight [g/mol]:	142.60
CAS:	10147-37-2

Physical Properties

Property code	Value	Unit	Source
gf	-508.53	kJ/mol	Joback Method
hf	-579.62	kJ/mol	Joback Method
hfus	15.58	kJ/mol	Joback Method
hvap	44.90	kJ/mol	Joback Method
log10ws	-1.17		Crippen Method
logp	0.963		Crippen Method
mcvol	93.460	ml/mol	McGowan Method
pc	5251.00	kPa	Joback Method
tb	352.81	K	Joback Method
tc	528.86	K	Joback Method
tf	177.05	K	Joback Method
vc	0.372	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	149.40	J/mol×K	352.81	Joback Method
cpg	156.77	J/mol×K	382.15	Joback Method
cpg	163.92	J/mol×K	411.49	Joback Method
cpg	170.83	J/mol×K	440.83	Joback Method
cpg	177.51	J/mol×K	470.18	Joback Method
cpg	183.95	J/mol×K	499.52	Joback Method

cpg	190.14	J/mol×K	528.86	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=C10147372&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