

1-Propanesulfonyl chloride

Other names:	Propane-1-sulfonyl chloride propanesulphonyl chloride
Inchi:	InChI=1S/C3H7ClO2S/c1-2-3-7(4,5)6/h2-3H2,1H3
InchiKey:	KPBSJEBFALFJTO-UHFFFAOYSA-N
Formula:	C3H7ClO2S
SMILES:	CCCS(=O)(=O)Cl
Mol. weight [g/mol]:	142.60
CAS:	10147-36-1

Physical Properties

Property code	Value	Unit	Source
gf	-506.09	kJ/mol	Joback Method
hf	-574.34	kJ/mol	Joback Method
hfus	19.10	kJ/mol	Joback Method
hvap	45.29	kJ/mol	Joback Method
log10ws	-1.06		Crippen Method
logp	0.965		Crippen Method
mvol	93.460	ml/mol	McGowan Method
pc	5190.64	kPa	Joback Method
tb	450.50 ± 2.50	K	NIST Webbook
tc	525.11	K	Joback Method
tf	192.05	K	Joback Method
vc	0.379	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	149.52	J/mol×K	353.25	Joback Method
cpg	156.62	J/mol×K	381.89	Joback Method
cpg	163.51	J/mol×K	410.54	Joback Method
cpg	170.19	J/mol×K	439.18	Joback Method
cpg	176.65	J/mol×K	467.83	Joback Method
cpg	182.88	J/mol×K	496.47	Joback Method
cpg	188.89	J/mol×K	525.11	Joback Method

hvapt	52.30	kJ/mol	317.50	NIST Webbook
hvapt	49.90	kJ/mol	413.00	NIST Webbook
hvapt	60.10	kJ/mol	258.00	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C10147361&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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
hvapt:	Enthalpy of vaporization at a given temperature
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

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