C10H13ClO2S

Inchi: InChI=1S/C10H13ClO2S/c1-6-5-7(2)9(4)10(8(6)3)14(11,12)13/h5H,1-4H3
InchiKey: ZCXRROBIIMQMHR-UHFFFAOYSA-N
Formula: C10H13ClO2S
SMILES: Cc1cc(C)c(C)c(S(=O)(=O)Cl)c1C
Mol. weight [g/mol]: 232.73
CAS: 60706-63-0

Physical Properties

Property code	Value	Unit	Source
gf	-373.26	kJ/mol	Joback Method
hf	-528.17	kJ/mol	Joback Method
hfus	29.72	kJ/mol	Joback Method
hvap	65.80	kJ/mol	Joback Method
log10ws	-3.79		Crippen Method
logp	2.848		Crippen Method
mcvol	168.330	ml/mol	McGowan Method
pc	3124.49	kPa	Joback Method
tb	560.01	K	Joback Method
tc	767.62	K	Joback Method
tf	347.44	K	Joback Method
vc	0.662	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	364.30	J/mol×K	560.01	Joback Method
cpg	377.52	J/mol×K	594.61	Joback Method
cpg	390.08	J/mol×K	629.21	Joback Method
cpg	401.98	J/mol×K	663.81	Joback Method
cpg	413.21	J/mol×K	698.41	Joback Method
cpg	423.77	J/mol×K	733.01	Joback Method
cpg	433.65	J/mol×K	767.62	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=C60706630&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

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