2-Mesitylenesulfonyl chloride

Other names:	2-Mesitylenesulfonyl chloride
	Mesitylenesulfonyl chloride
	Mesitylsulfonyl chloride
	2,4,6-Trimethylbenzenesulfonyl chloride
	mesitylene-2-sulphonyl chloride
Inchi:	InChI=1S/C9H11ClO2S/c1-6-4-7(2)9(8(3)5-6)13(10,11)12/h4-5H,1-3H3
InchiKey:	PVJZBZSCGJAWNG-UHFFFAOYSA-N
Formula:	C9H11ClO2S
SMILES:	Cc1cc(C)c(S(=O)(=O)Cl)c(C)c1
Mol. weight [g/mol]:	218.71

Physical Properties

Property code	Value	Unit	Source
af	0.5444		Cheméo Relay (1.0)
gf	-372.05	kJ/mol	Joback Method
hf	-341.84	kJ/mol	Cheméo Relay (1.0)
hfus	27.52	kJ/mol	Joback Method
hvap	72.91	kJ/mol	Cheméo Relay (1.0)
ie	8.95	eV	Cheméo Relay (1.0)
logp	2.539		Crippen Method
mcvol	154.240	ml/mol	McGowan Method
pc	3551.53	kPa	Joback Method
tb	555.88	K	Cheméo Relay (1.0)
tc	804.67	K	Cheméo Relay (1.0)
tf	342.11	K	Cheméo Relay (1.0)
vc	0.540	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	319.27	J/mol×K	532.15	Joback Method
cpg	331.84	J/mol×K	567.12	Joback Method
cpg	343.77	J/mol×K	602.09	Joback Method
cpg	355.05	J/mol×K	637.06	Joback Method

cpg	365.68	J/mol×K	672.04	Joback Method
cpg	375.67	J/mol×K	707.01	Joback Method
cpg	385.00	J/mol×K	741.98	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C773648&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

af:	Acentric Factor
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
ie:	Ionization energy
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