4-(methylsulfonyl)benzaldehyde

Inchi: InChI=1S/C8H8O3S/c1-12(10,11)8-4-2-7(6-9)3-5-8/h2-6H,1H3
InchiKey: PSVPUHBSBYJSMQ-UHFFFAOYSA-N
Formula: C8H8O3S
SMILES: CS(=O)(=O)c1ccc(C=O)cc1
Mol. weight [g/mol]: 184.22

Physical Properties

Property code	Value	Unit	Source
af	0.5423		Cheméo Relay (1.0)
gf	-448.80	kJ/mol	Joback Method
hf	-368.32	kJ/mol	Cheméo Relay (1.0)
hfus	26.19	kJ/mol	Solubility Modeling of 4-(Methylsulfonyl)benzaldehyde in Nine Organic Solvents at Elevated Temperatures
hvap	99.26	kJ/mol	Cheméo Relay (1.0)
ie	9.94	eV	Cheméo Relay (1.0)
log10ws	-2.06		Cheméo Relay (1.0)
logp	0.903		Crippen Method
mcvol	129.480	ml/mol	McGowan Method
pc	4815.84	kPa	Joback Method
tb	601.63	K	Cheméo Relay (1.0)
tc	845.44	K	Cheméo Relay (1.0)
tf	410.88	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	267.68	J/mol×K	510.54	Joback Method
cpg	279.21	J/mol×K	545.49	Joback Method
cpg	290.07	J/mol×K	580.45	Joback Method
cpg	300.27	J/mol×K	615.40	Joback Method
cpg	309.82	J/mol×K	650.35	Joback Method
cpg	318.73	J/mol×K	685.31	Joback Method
cpg	326.99	J/mol×K	720.26	Joback Method

Sources

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
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
Solubility Modeling of 4-(Methylsulfonyl)benzaldehyde in Nine Organic Solvents at Elevated Temperatures:	https://www.doi.org/10.1021/acs.jced.5b01053

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
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