3-Cl-4-CH3S-C6H3-CCH

Inchi: InChI=1S/C9H7ClS/c1-3-7-4-5-9(11-2)8(10)6-7/h1,4-6H,2H3
InchiKey: YMRAHBGPMBCMLR-UHFFFAOYSA-N
Formula: C9H7ClS
SMILES: C#Cc1ccc(SC)c(Cl)c1
Mol. weight [g/mol]: 182.67
CAS: 120136-30-3

Physical Properties

Property code	Value	Unit	Source
affp	868.60	kJ/mol	NIST Webbook
basg	836.10	kJ/mol	NIST Webbook
gf	362.31	kJ/mol	Joback Method
hf	302.53	kJ/mol	Joback Method
hfus	23.63	kJ/mol	Joback Method
hvap	50.29	kJ/mol	Joback Method
log10ws	-3.60		Crippen Method
logp	3.043		Crippen Method
mcvol	133.900	ml/mol	McGowan Method
pc	3659.77	kPa	Joback Method
tb	538.29	K	Joback Method
tc	795.02	K	Joback Method
tf	353.94	K	Joback Method
vc	0.496	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	254.42	J/mol×K	538.29	Joback Method
cpg	265.37	J/mol×K	581.08	Joback Method
cpg	275.53	J/mol×K	623.87	Joback Method
cpg	284.94	J/mol×K	666.65	Joback Method
cpg	293.63	J/mol×K	709.44	Joback Method
cpg	301.63	J/mol×K	752.23	Joback Method
cpg	308.98	J/mol×K	795.02	Joback Method

Sources

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=C120136303&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

affp:	Proton affinity
basg:	Gas basicity
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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