4-CH3S-C6H4-CCH

Inchi: InChI=1S/C9H8S/c1-3-8-4-6-9(10-2)7-5-8/h1,4-7H,2H3
InchiKey: LLDBWBLRNOTXLL-UHFFFAOYSA-N
Formula: C9H8S
SMILES: C#Cc1ccc(SC)cc1
Mol. weight [g/mol]: 148.22
CAS: 56041-85-1

Physical Properties

Property code	Value	Unit	Source
affp	886.60	kJ/mol	NIST Webbook
basg	854.10	kJ/mol	NIST Webbook
gf	383.87	kJ/mol	Joback Method
hf	329.74	kJ/mol	Joback Method
hfus	19.82	kJ/mol	Joback Method
hvap	45.24	kJ/mol	Joback Method
log10ws	-2.91		Crippen Method
logp	2.390		Crippen Method
mcvol	121.660	ml/mol	McGowan Method
pc	3901.37	kPa	Joback Method
tb	495.88	K	Joback Method
tc	746.36	K	Joback Method
tf	311.50	K	Joback Method
vc	0.448	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	232.18	J/mol×K	495.88	Joback Method
cpg	244.38	J/mol×K	537.63	Joback Method
cpg	255.73	J/mol×K	579.37	Joback Method
cpg	266.26	J/mol×K	621.12	Joback Method
cpg	276.02	J/mol×K	662.87	Joback Method
cpg	285.03	J/mol×K	704.62	Joback Method
cpg	293.35	J/mol×K	746.36	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=C56041851&Units=SI

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