Carbon disulfide cation

Inchi: InChI=1S/CS2/c2-1-3/q+1
InchiKey: PGXKVSYXGLLKDQ-UHFFFAOYSA-N
Formula: CS2
SMILES: S=[C+]=S
Mol. weight [g/mol]: 76.14
CAS: 12539-80-9

Physical Properties

Property code	Value	Unit	Source
gf	256.82	kJ/mol	Joback Method
hf	294.17	kJ/mol	Joback Method
hfus	12.10	kJ/mol	Joback Method
hvap	31.60	kJ/mol	Joback Method
log10ws	-1.37		Crippen Method
logp	1.018		Crippen Method
mcvol	49.050	ml/mol	McGowan Method
pc	8264.46	kPa	Joback Method
tb	361.71	K	Joback Method
tc	594.16	K	Joback Method
tf	209.08	K	Joback Method
vc	0.162	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	57.76	J/mol×K	361.71	Joback Method
cpg	58.82	J/mol×K	400.45	Joback Method
cpg	59.60	J/mol×K	439.19	Joback Method
cpg	60.16	J/mol×K	477.93	Joback Method
cpg	60.52	J/mol×K	516.67	Joback Method
cpg	60.72	J/mol×K	555.42	Joback Method
cpg	60.79	J/mol×K	594.16	Joback Method

Sources

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=C12539809&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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