Methyl dithioacetate

Inchi: InChI=1S/C3H6S2/c1-3(4)5-2/h1-2H3
InchiKey: PFWSEYMNCOMKDX-UHFFFAOYSA-N
Formula: C3H6S2
SMILES: CSC(C)=S
Mol. weight [g/mol]: 106.21
CAS: 2168-84-5

Physical Properties

Property code	Value	Unit	Source
affp	860.70	kJ/mol	NIST Webbook
basg	831.50	kJ/mol	NIST Webbook
gf	124.56	kJ/mol	Joback Method
hf	83.12	kJ/mol	Joback Method
hfus	12.26	kJ/mol	Joback Method
hvap	35.82	kJ/mol	Joback Method
ie	8.10	eV	NIST Webbook
ie	8.50	eV	NIST Webbook
log10ws	-1.81		Crippen Method
logp	1.697		Crippen Method
mcvol	81.530	ml/mol	McGowan Method
pc	5123.98	kPa	Joback Method
rinpol	831.00		NIST Webbook
tb	406.86	K	Joback Method
tc	634.32	K	Joback Method
tf	192.24	K	Joback Method
vc	0.293	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	126.65	J/mol×K	406.86	Joback Method
cpg	133.56	J/mol×K	444.77	Joback Method
cpg	139.98	J/mol×K	482.68	Joback Method
cpg	145.93	J/mol×K	520.59	Joback Method

cpg	151.46	J/mol×K	558.50	Joback Method
cpg	156.59	J/mol×K	596.41	Joback Method
cpg	161.36	J/mol×K	634.32	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=C2168845&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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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