2,4,5-Trimethyl-[1,3]dithiole

Inchi: InChI=1S/C6H12S2/c1-4-5(2)8-6(3)7-4/h4-6H,1-3H3
InchiKey: CEEIENLFRSOFRE-UHFFFAOYSA-N
Formula: C6H12S2
SMILES: CC1SC(C)C(C)S1
Mol. weight [g/mol]: 148.29

Physical Properties

Property code	Value	Unit	Source
gf	100.49	kJ/mol	Joback Method
hf	-56.85	kJ/mol	Joback Method
hfus	14.69	kJ/mol	Joback Method
hvap	40.21	kJ/mol	Joback Method
log10ws	-2.83		Crippen Method
logp	2.589		Crippen Method
mcvol	117.240	ml/mol	McGowan Method
pc	3493.01	kPa	Joback Method
ripol	1586.00		NIST Webbook
ripol	1586.00		NIST Webbook
tb	438.28	K	Joback Method
tc	667.13	K	Joback Method
tf	326.70	K	Joback Method
vc	0.403	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	227.73	J/mol×K	438.28	Joback Method
cpg	242.74	J/mol×K	476.42	Joback Method
cpg	256.96	J/mol×K	514.56	Joback Method
cpg	270.42	J/mol×K	552.70	Joback Method
cpg	283.13	J/mol×K	590.84	Joback Method
cpg	295.12	J/mol×K	628.99	Joback Method
cpg	306.41	J/mol×K	667.13	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R494996&Units=SI
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

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume