3,5-Dimethyl-[1,2,4]trithiolane, stereoisomer 2

Inchi: InChI=1S/C4H8S3/c1-3-5-4(2)7-6-3/h3-4H,1-2H3
InchiKey: HFRUNLRFNNTTPQ-UHFFFAOYSA-N
Formula: C4H8S3
SMILES: CC1SSC(C)S1
Mol. weight [g/mol]: 152.30

Physical Properties

Property code	Value	Unit	Source
gf	131.22	kJ/mol	Joback Method
hf	50.03	kJ/mol	Joback Method
hfus	12.09	kJ/mol	Joback Method
hvap	41.88	kJ/mol	Joback Method
log10ws	-3.25		Crippen Method
logp	2.807		Crippen Method
mcvol	105.410	ml/mol	McGowan Method
pc	4608.87	kPa	Joback Method
ripol	1560.00		NIST Webbook
tb	445.02	K	Joback Method
tc	698.77	K	Joback Method
tf	391.85	K	Joback Method
vc	0.338	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	189.82	J/mol×K	445.02	Joback Method
cpg	201.68	J/mol×K	487.31	Joback Method
cpg	212.78	J/mol×K	529.60	Joback Method
cpg	223.15	J/mol×K	571.90	Joback Method
cpg	232.82	J/mol×K	614.19	Joback Method
cpg	241.83	J/mol×K	656.48	Joback Method
cpg	250.21	J/mol×K	698.77	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=R495177&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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