1,2,4-Trithiolane, 3,5-dimethyl, #2

Other names: 3,5-dimethyl-1,2,4-trithiolane, B
syn-3,5-dimethyl-1,2,4-trithiolane
Inchi: InChI=1S/C4H8S3/c1-3-5-4(2)7-6-3/h3-4H,1-2H3/t3-,4+
InchiKey: HFRUNLRFNNTTPQ-ZXZARUISSA-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
rinpol	1107.00		NIST Webbook
rinpol	1154.00		NIST Webbook
rinpol	1108.00		NIST Webbook
rinpol	1106.00		NIST Webbook
rinpol	1181.00		NIST Webbook
rinpol	1127.00		NIST Webbook
rinpol	1154.00		NIST Webbook
rinpol	1177.00		NIST Webbook
rinpol	1144.00		NIST Webbook
rinpol	1151.00		NIST Webbook
rinpol	1110.00		NIST Webbook
rinpol	1169.00		NIST Webbook
ripol	1586.00		NIST Webbook
ripol	1578.00		NIST Webbook
ripol	1588.00		NIST Webbook
ripol	1588.00		NIST Webbook
ripol	1603.00		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

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=R44633&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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices

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