1,2,4-TRITHIOLANE

Inchi: InChI=1S/C2H4S3/c1-3-2-5-4-1/h1-2H2
InchiKey: QHGFEUAAQKJXDI-UHFFFAOYSA-N
Formula: C2H4S3
SMILES: C1SCSS1
Mol. weight [g/mol]: 124.25

Physical Properties

Property code	Value	Unit	Source
hfus	4.77	kJ/mol	Joback Method
ie	8.70 ± 0.20	eV	NIST Webbook
ie	8.72	eV	NIST Webbook
logp	2.030		Crippen Method
mcvol	77.230	ml/mol	McGowan Method
rinpol	1065.00		NIST Webbook
rinpol	1127.00		NIST Webbook
rinpol	1073.00		NIST Webbook
rinpol	1106.00		NIST Webbook
rinpol	1107.00		NIST Webbook
rinpol	1107.00		NIST Webbook
rinpol	1127.00		NIST Webbook
rinpol	1073.00		NIST Webbook
ripol	1760.00		NIST Webbook
ripol	1760.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	114.80	J/mol×K	408.60	Joback Method
cpg	122.51	J/mol×K	452.48	Joback Method
cpg	129.53	J/mol×K	496.36	Joback Method
cpg	135.92	J/mol×K	540.24	Joback Method
cpg	141.72	J/mol×K	584.12	Joback Method
cpg	147.00	J/mol×K	628.00	Joback Method
cpg	151.80	J/mol×K	671.88	Joback Method

Sources

Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C289167&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
ripol:	Polar retention indices