Trisulfide, diethyl

Other names:	Diethyl trisulfide
	Ethyl trisulfide
	3,4,5-Trithiaheptane
	NSC 97329
	diethyl trisulphide
Inchi:	InChI=1S/C4H10S3/c1-3-5-7-6-4-2/h3-4H2,1-2H3
InchiKey:	OPMRTBDRQRSNDN-UHFFFAOYSA-N
Formula:	C4H10S3
SMILES:	CCSSSCC
Mol. weight [g/mol]:	154.32
CAS:	3600-24-6

Physical Properties

Property code	Value	Unit	Source
gf	82.16	kJ/mol	Joback Method
hf	-0.28	kJ/mol	Joback Method
hfus	18.51	kJ/mol	Joback Method
hvap	44.95	kJ/mol	Joback Method
log10ws	-3.13		Crippen Method
logp	3.056		Crippen Method
mcvol	116.270	ml/mol	McGowan Method
pc	4156.97	kPa	Joback Method
rinpol	1132.00		NIST Webbook
rinpol	1140.00		NIST Webbook
rinpol	1125.00		NIST Webbook
rinpol	1132.00		NIST Webbook
rinpol	1129.00		NIST Webbook
rinpol	1129.00		NIST Webbook
rinpol	1125.00		NIST Webbook
rinpol	1157.00		NIST Webbook
rinpol	1140.00		NIST Webbook
ripol	1520.00		NIST Webbook
ripol	1520.00		NIST Webbook
tb	497.26	K	Joback Method
tc	740.19	K	Joback Method
tf	238.04	K	Joback Method
vc	0.421	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	216.75	J/mol×K	497.26	Joback Method
cpg	227.03	J/mol×K	537.75	Joback Method
cpg	236.83	J/mol×K	578.24	Joback Method
cpg	246.12	J/mol×K	618.73	Joback Method
cpg	254.89	J/mol×K	659.22	Joback Method
cpg	263.12	J/mol×K	699.70	Joback Method
cpg	270.79	J/mol×K	740.19	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=C3600246&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