Methyl pentyl trisulfide

Inchi: InChI=1S/C6H14S3/c1-3-4-5-6-8-9-7-2/h3-6H2,1-2H3
InchiKey: FOEDHONXFISGJF-UHFFFAOYSA-N
Formula: C6H14S3
SMILES: CCCCCSSSC
Mol. weight [g/mol]: 182.37

Physical Properties

Property code	Value	Unit	Source
gf	99.00	kJ/mol	Joback Method
hf	-41.56	kJ/mol	Joback Method
hfus	23.69	kJ/mol	Joback Method
hvap	49.40	kJ/mol	Joback Method
log10ws	-3.97		Crippen Method
logp	3.836		Crippen Method
mcvol	144.450	ml/mol	McGowan Method
pc	3291.59	kPa	Joback Method
rinpol	1376.00		NIST Webbook
tb	543.02	K	Joback Method
tc	776.68	K	Joback Method
tf	260.58	K	Joback Method
vc	0.533	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	301.42	J/mol×K	543.02	Joback Method
cpg	314.30	J/mol×K	581.96	Joback Method
cpg	326.51	J/mol×K	620.91	Joback Method
cpg	338.04	J/mol×K	659.85	Joback Method
cpg	348.88	J/mol×K	698.79	Joback Method
cpg	359.03	J/mol×K	737.73	Joback Method
cpg	368.48	J/mol×K	776.68	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R502720&Units=SI

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

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