Methyl neopentyl disulfide

Inchi: InChI=1S/C6H14S2/c1-6(2,3)5-8-7-4/h5H2,1-4H3
InchiKey: UUFBJRBAPHQZBB-UHFFFAOYSA-N
Formula: C6H14S2
SMILES: CSSCC(C)(C)C
Mol. weight [g/mol]: 150.31

Physical Properties

Property code	Value	Unit	Source
gf	68.72	kJ/mol	Joback Method
hf	-92.18	kJ/mol	Joback Method
hfus	12.14	kJ/mol	Joback Method
hvap	41.29	kJ/mol	Joback Method
log10ws	-2.85		Crippen Method
logp	3.044		Crippen Method
mcvol	128.100	ml/mol	McGowan Method
pc	3299.15	kPa	Joback Method
rinpol	1072.00		NIST Webbook
rinpol	1072.00		NIST Webbook
ripol	1268.00		NIST Webbook
ripol	1268.00		NIST Webbook
tb	471.01	K	Joback Method
tc	697.89	K	Joback Method
tf	228.60	K	Joback Method
vc	0.469	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	257.06	J/mol×K	471.01	Joback Method
cpg	270.59	J/mol×K	508.82	Joback Method
cpg	283.33	J/mol×K	546.64	Joback Method
cpg	295.30	J/mol×K	584.45	Joback Method
cpg	306.53	J/mol×K	622.27	Joback Method
cpg	317.05	J/mol×K	660.08	Joback Method

cpg	326.87	J/mol×K	697.89	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=R602390&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
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