methyl isopentenyl disulfide

Inchi: InChI=1S/C6H12S2/c1-6(2)4-5-8-7-3/h4H,5H2,1-3H3
InchiKey: IUWTWUFCWBZDLR-UHFFFAOYSA-N
Formula: C6H12S2
SMILES: CSSCC=C(C)C
Mol. weight [g/mol]: 148.29

Physical Properties

Property code	Value	Unit	Source
gf	137.55	kJ/mol	Joback Method
hf	24.00	kJ/mol	Joback Method
hfus	18.45	kJ/mol	Joback Method
hvap	42.62	kJ/mol	Joback Method
log10ws	-2.95		Crippen Method
logp	2.964		Crippen Method
mcvol	123.800	ml/mol	McGowan Method
pc	3448.03	kPa	Joback Method
rinpol	1093.00		NIST Webbook
rinpol	1093.00		NIST Webbook
tb	478.28	K	Joback Method
tc	705.69	K	Joback Method
tf	207.14	K	Joback Method
vc	0.461	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	236.78	J/mol×K	478.28	Joback Method
cpg	248.77	J/mol×K	516.18	Joback Method
cpg	260.11	J/mol×K	554.08	Joback Method
cpg	270.82	J/mol×K	591.98	Joback Method
cpg	280.92	J/mol×K	629.88	Joback Method
cpg	290.43	J/mol×K	667.79	Joback Method
cpg	299.37	J/mol×K	705.69	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R493037&Units=SI
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

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