1-Propene, 1-(methylthio)-, (E)-

Inchi: InChI=1S/C4H8S/c1-3-4-5-2/h3-4H,1-2H3/b4-3+
InchiKey: YJOGCMRDEUBRJD-ONEGZZNKSA-N
Formula: C4H8S
SMILES: CC=CSC
Mol. weight [g/mol]: 88.17
CAS: 42848-06-6

Physical Properties

Property code	Value	Unit	Source
gf	96.14	kJ/mol	Joback Method
hf	33.20	kJ/mol	Joback Method
hfus	10.45	kJ/mol	Joback Method
hvap	31.27	kJ/mol	Joback Method
log10ws	-1.73		Crippen Method
logp	1.883		Crippen Method
mcvol	79.270	ml/mol	McGowan Method
pc	4255.16	kPa	Joback Method
rinpol	726.00		NIST Webbook
rinpol	678.00		NIST Webbook
rinpol	684.00		NIST Webbook
rinpol	726.00		NIST Webbook
tb	363.86	K	Joback Method
tc	565.66	K	Joback Method
tf	164.16	K	Joback Method
vc	0.293	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	120.85	J/mol×K	363.86	Joback Method
cpg	128.98	J/mol×K	397.49	Joback Method
cpg	136.74	J/mol×K	431.13	Joback Method
cpg	144.11	J/mol×K	464.76	Joback Method
cpg	151.13	J/mol×K	498.39	Joback Method

cpg	157.81	J/mol×K	532.03	Joback Method
cpg	164.14	J/mol×K	565.66	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C42848066&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

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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