trans-1-(Methylthio)-2-butene

Inchi: InChI=1S/C5H10S/c1-3-4-5-6-2/h3-4H,5H2,1-2H3/b4-3+
InchiKey: QPUBNJBEYGHVGN-ONEGZZNKSA-N
Formula: C5H10S
SMILES: CC=CCSC
Mol. weight [g/mol]: 102.20
CAS: 4088-54-4

Physical Properties

Property code	Value	Unit	Source
gf	104.56	kJ/mol	Joback Method
hf	12.56	kJ/mol	Joback Method
hfus	13.04	kJ/mol	Joback Method
hvap	33.50	kJ/mol	Joback Method
log10ws	-1.65		Crippen Method
logp	1.925		Crippen Method
mcvol	93.360	ml/mol	McGowan Method
pc	3768.41	kPa	Joback Method
tb	386.74	K	Joback Method
tc	587.18	K	Joback Method
tf	175.43	K	Joback Method
vc	0.349	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	154.81	J/mol×K	386.74	Joback Method
cpg	164.53	J/mol×K	420.15	Joback Method
cpg	173.79	J/mol×K	453.55	Joback Method
cpg	182.61	J/mol×K	486.96	Joback Method
cpg	191.00	J/mol×K	520.37	Joback Method
cpg	198.98	J/mol×K	553.77	Joback Method
cpg	206.56	J/mol×K	587.18	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=C4088544&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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