Butanoic acid, 4-(methylthio)-

Other names: 4-methylthiobutanoic acid
Inchi: InChI=1S/C5H10O2S/c1-8-4-2-3-5(6)7/h2-4H2,1H3,(H,6,7)
InchiKey: VDSUAILXEZKWIZ-UHFFFAOYSA-N
Formula: C5H10O2S
SMILES: CSCCCC(=O)O
Mol. weight [g/mol]: 134.20
CAS: 32391-97-2

Physical Properties

Property code	Value	Unit	Source
gf	-241.40	kJ/mol	Joback Method
hf	-369.47	kJ/mol	Joback Method
hfus	18.52	kJ/mol	Joback Method
hvap	56.97	kJ/mol	Joback Method
log10ws	-0.90		Crippen Method
logp	1.214		Crippen Method
mcvol	105.100	ml/mol	McGowan Method
pc	4294.29	kPa	Joback Method
ripol	2384.00		NIST Webbook
ripol	2384.00		NIST Webbook
tb	528.63	K	Joback Method
tc	720.17	K	Joback Method
tf	291.26	K	Joback Method
vc	0.395	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	225.69	J/mol×K	528.63	Joback Method
cpg	233.96	J/mol×K	560.55	Joback Method
cpg	241.86	J/mol×K	592.48	Joback Method
cpg	249.38	J/mol×K	624.40	Joback Method
cpg	256.54	J/mol×K	656.32	Joback Method
cpg	263.34	J/mol×K	688.25	Joback Method

cpg	269.77	J/mol×K	720.17	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=C32391972&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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