

Methyl 4-(methylthio)butyrate

Other names:	Butanoic acid, 4-(methylthio)-, methyl ester Methyl 4-(methylthio)butanoate
Inchi:	InChI=1S/C6H12O2S/c1-8-6(7)4-3-5-9-2/h3-5H2,1-2H3
InchiKey:	HQDLZISNHUMXEA-UHFFFAOYSA-N
Formula:	C6H12O2S
SMILES:	COC(=O)CCCSC
Mol. weight [g/mol]:	148.22
CAS:	53053-51-3

Physical Properties

Property code	Value	Unit	Source
gf	-201.16	kJ/mol	Joback Method
hf	-370.10	kJ/mol	Joback Method
hfus	18.21	kJ/mol	Joback Method
hvap	44.92	kJ/mol	Joback Method
log10ws	-1.08		Crippen Method
logp	1.303		Crippen Method
mcvol	119.190	ml/mol	McGowan Method
pc	3337.38	kPa	Joback Method
rinpol	1098.00		NIST Webbook
rinpol	1098.00		NIST Webbook
ripol	1636.00		NIST Webbook
ripol	1617.00		NIST Webbook
tb	481.75	K	Joback Method
tc	681.10	K	Joback Method
tf	263.94	K	Joback Method
vc	0.450	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	245.41	J/molxK	481.75	Joback Method
cpg	256.09	J/molxK	514.98	Joback Method
cpg	266.37	J/molxK	548.20	Joback Method

cpg	276.25	J/mol×K	581.43	Joback Method
cpg	285.71	J/mol×K	614.65	Joback Method
cpg	294.75	J/mol×K	647.88	Joback Method
cpg	303.37	J/mol×K	681.10	Joback Method

Sources

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=C53053513&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

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

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