

3-methylbutyl 3-(methylthio)propanoate

Inchi:	InChI=1S/C9H18O2S/c1-8(2)4-6-11-9(10)5-7-12-3/h8H,4-7H2,1-3H3
InchiKey:	UUBYGRBYGZQQQG-UHFFFAOYSA-N
Formula:	C9H18O2S
SMILES:	CSCCC(=O)OCCC(C)C
Mol. weight [g/mol]:	190.30

Physical Properties

Property code	Value	Unit	Source
gf	-178.34	kJ/mol	Joback Method
hf	-437.30	kJ/mol	Joback Method
hfus	22.46	kJ/mol	Joback Method
hvap	51.21	kJ/mol	Joback Method
log10ws	-2.09		Crippen Method
logp	2.329		Crippen Method
mcvol	161.460	ml/mol	McGowan Method
pc	2472.73	kPa	Joback Method
ripol	1792.00		NIST Webbook
tb	549.95	K	Joback Method
tc	745.63	K	Joback Method
tf	282.75	K	Joback Method
vc	0.612	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	378.02	J/molxK	549.95	Joback Method
cpg	392.14	J/molxK	582.56	Joback Method
cpg	405.64	J/molxK	615.18	Joback Method
cpg	418.52	J/molxK	647.79	Joback Method
cpg	430.78	J/molxK	680.40	Joback Method
cpg	442.42	J/molxK	713.02	Joback Method
cpg	453.44	J/molxK	745.63	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=R327118&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.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
hvac:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccol:	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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