3-(1-Methyl-3-oxo-propylsulfanyl)-butyraldehyde

Inchi: InChI=1S/C8H14O2S/c1-7(3-5-9)11-8(2)4-6-10/h5-8H,3-4H2,1-2H3
InchiKey: HPRLAICEPOYLIX-UHFFFAOYSA-N
Formula: C8H14O2S
SMILES: CC(CC=O)SC(C)CC=O
Mol. weight [g/mol]: 174.26

Physical Properties

Property code	Value	Unit	Source
gf	-154.32	kJ/mol	Joback Method
hf	-348.30	kJ/mol	Joback Method
hfus	18.14	kJ/mol	Joback Method
hvap	52.88	kJ/mol	Joback Method
log10ws	-1.84		Crippen Method
logp	1.675		Crippen Method
mcvol	143.070	ml/mol	McGowan Method
pc	3069.34	kPa	Joback Method
rinpol	1288.00		NIST Webbook
rinpol	1288.00		NIST Webbook
tb	547.66	K	Joback Method
tc	751.05	K	Joback Method
tf	268.32	K	Joback Method
vc	0.559	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	327.79	J/mol×K	547.66	Joback Method
cpg	339.91	J/mol×K	581.56	Joback Method
cpg	351.39	J/mol×K	615.46	Joback Method
cpg	362.26	J/mol×K	649.36	Joback Method
cpg	372.52	J/mol×K	683.25	Joback Method
cpg	382.19	J/mol×K	717.15	Joback Method
cpg	391.27	J/mol×K	751.05	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R487295&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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