3-(2-Oxobutyldithio)butan-2-one

Inchi: InChI=1S/C8H14O2S2/c1-4-8(10)5-11-12-7(3)6(2)9/h7H,4-5H2,1-3H3
InchiKey: PPDLAKNOOLOHTR-UHFFFAOYSA-N
Formula: C8H14O2S2
SMILES: CCC(=O)CSSC(C)C(C)=O
Mol. weight [g/mol]: 206.33

Physical Properties

Property code	Value	Unit	Source
gf	-177.56	kJ/mol	Joback Method
hf	-355.15	kJ/mol	Joback Method
hfus	24.41	kJ/mol	Joback Method
hvap	60.14	kJ/mol	Joback Method
log10ws	-2.60		Crippen Method
logp	2.324		Crippen Method
mcvol	159.420	ml/mol	McGowan Method
pc	3025.61	kPa	Joback Method
rinpol	1547.00		NIST Webbook
rinpol	1547.00		NIST Webbook
tb	627.30	K	Joback Method
tc	853.59	K	Joback Method
tf	333.58	K	Joback Method
vc	0.598	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	374.29	J/mol×K	627.30	Joback Method
cpg	386.80	J/mol×K	665.02	Joback Method
cpg	398.53	J/mol×K	702.73	Joback Method
cpg	409.47	J/mol×K	740.45	Joback Method
cpg	419.63	J/mol×K	778.16	Joback Method
cpg	429.02	J/mol×K	815.88	Joback Method
cpg	437.64	J/mol×K	853.59	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R90626&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