2-oxopropyl 3-oxo-2-butyl disulfide

Inchi: InChI=1S/C7H12O2S2/c1-5(8)4-10-11-7(3)6(2)9/h7H,4H2,1-3H3
InchiKey: HNFHHSMMXNNSFS-UHFFFAOYSA-N
Formula: C7H12O2S2
SMILES: CC(=O)CSSC(C)C(C)=O
Mol. weight [g/mol]: 192.30

Physical Properties

Property code	Value	Unit	Source
gf	-185.98	kJ/mol	Joback Method
hf	-334.51	kJ/mol	Joback Method
hfus	21.82	kJ/mol	Joback Method
hvap	57.91	kJ/mol	Joback Method
log10ws	-2.18		Crippen Method
logp	1.934		Crippen Method
mcvol	145.330	ml/mol	McGowan Method
pc	3372.36	kPa	Joback Method
rinpol	1436.00		NIST Webbook
rinpol	1436.00		NIST Webbook
ripol	2280.00		NIST Webbook
ripol	2280.00		NIST Webbook
tb	604.42	K	Joback Method
tc	835.16	K	Joback Method
tf	322.31	K	Joback Method
vc	0.541	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	327.04	J/mol×K	604.42	Joback Method
cpg	338.71	J/mol×K	642.88	Joback Method
cpg	349.64	J/mol×K	681.33	Joback Method
cpg	359.85	J/mol×K	719.79	Joback Method
cpg	369.33	J/mol×K	758.24	Joback Method
cpg	378.08	J/mol×K	796.70	Joback Method

cpg	386.10	J/mol×K	835.16	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R224123&Units=SI

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