bis(1-methyl-2-oxobutyl) sulfide

Inchi: InChI=1S/C10H18O2S/c1-5-9(11)7(3)13-8(4)10(12)6-2/h7-8H,5-6H2,1-4H3
InchiKey: STEMUDBXFWZOOG-UHFFFAOYSA-N
Formula: C10H18O2S
SMILES: CCC(=O)C(C)SC(C)C(=O)CC
Mol. weight [g/mol]: 202.31

Physical Properties

Property code	Value	Unit	Source
gf	-196.28	kJ/mol	Joback Method
hf	-443.58	kJ/mol	Joback Method
hfus	21.94	kJ/mol	Joback Method
hvap	57.39	kJ/mol	Joback Method
log10ws	-2.68		Crippen Method
logp	2.455		Crippen Method
mcvol	171.250	ml/mol	McGowan Method
pc	2453.17	kPa	Joback Method
rinpol	1460.00		NIST Webbook
rinpol	1460.00		NIST Webbook
tb	603.84	K	Joback Method
tc	810.31	K	Joback Method
tf	306.72	K	Joback Method
vc	0.649	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	420.41	J/mol×K	603.84	Joback Method
cpg	434.76	J/mol×K	638.25	Joback Method
cpg	448.33	J/mol×K	672.66	Joback Method
cpg	461.12	J/mol×K	707.07	Joback Method
cpg	473.16	J/mol×K	741.49	Joback Method
cpg	484.46	J/mol×K	775.90	Joback Method
cpg	495.03	J/mol×K	810.31	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=R223100&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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