bis(1-methyl-2-oxobutyl)trisulfide

Inchi: InChI=1S/C10H18O2S3/c1-5-9(11)7(3)13-15-14-8(4)10(12)6-2/h7-8H,5-6H2,1-4H3
InchiKey: PCGMQMBQFGENKJ-UHFFFAOYSA-N
Formula: C10H18O2S3
SMILES: CCC(=O)C(C)SSSC(C)C(=O)CC
Mol. weight [g/mol]: 266.44

Physical Properties

Property code	Value	Unit	Source
gf	-130.04	kJ/mol	Joback Method
hf	-359.84	kJ/mol	Joback Method
hfus	30.20	kJ/mol	Joback Method
hvap	71.02	kJ/mol	Joback Method
log10ws	-4.42		Crippen Method
logp	3.751		Crippen Method
mcvol	203.950	ml/mol	McGowan Method
pc	2537.93	kPa	Joback Method
rinpol	1899.00		NIST Webbook
rinpol	1899.00		NIST Webbook
tb	741.40	K	Joback Method
tc	978.92	K	Joback Method
tf	375.52	K	Joback Method
vc	0.757	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	525.71	J/mol×K	741.40	Joback Method
cpg	539.25	J/mol×K	780.99	Joback Method
cpg	551.68	J/mol×K	820.57	Joback Method
cpg	562.99	J/mol×K	860.16	Joback Method
cpg	573.20	J/mol×K	899.74	Joback Method
cpg	582.31	J/mol×K	939.33	Joback Method
cpg	590.31	J/mol×K	978.92	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R223115&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