

bis(1-methyl-2-oxopropyl) disulfide

Other names:	bis(3-oxo-2-butyl) disulfide
Inchi:	InChI=1S/C8H14O2S2/c1-5(9)7(3)11-12-8(4)6(2)10/h7-8H,1-4H3
InchiKey:	NLXBKJGCEKRYJY-UHFFFAOYSA-N
Formula:	C8H14O2S2
SMILES:	CC(=O)C(C)SSC(C)C(C)=O
Mol. weight [g/mol]:	206.33

Physical Properties

Property code	Value	Unit	Source
gf	-180.00	kJ/mol	Joback Method
hf	-360.43	kJ/mol	Joback Method
hfus	20.89	kJ/mol	Joback Method
hvap	59.75	kJ/mol	Joback Method
log10ws	-2.71		Crippen Method
logp	2.323		Crippen Method
mcvol	159.420	ml/mol	McGowan Method
pc	3052.41	kPa	Joback Method
rinpol	1460.00		NIST Webbook
rinpol	1478.00		NIST Webbook
rinpol	1478.00		NIST Webbook
rinpol	1489.00		NIST Webbook
rinpol	1460.00		NIST Webbook
rinpol	1476.00		NIST Webbook
ripol	2204.00		NIST Webbook
ripol	2204.00		NIST Webbook
tb	626.86	K	Joback Method
tc	857.93	K	Joback Method
tf	318.58	K	Joback Method
vc	0.592	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	374.78	J/mol×K	626.86	Joback Method

cpg	387.61	J/mol×K	665.37	Joback Method
cpg	399.60	J/mol×K	703.88	Joback Method
cpg	410.76	J/mol×K	742.40	Joback Method
cpg	421.10	J/mol×K	780.91	Joback Method
cpg	430.61	J/mol×K	819.42	Joback Method
cpg	439.30	J/mol×K	857.93	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=R222929&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
mvol:	McGowan's characteristic volume
pc:	Critical Pressure
ripol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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