

Dimethyl 3-thiaadipate

Other names:	Propanoic acid, 3-[(2-methoxy-2-oxoethyl)thio]-, methyl ester Methyl 3-(methoxycarbonylmethylthio)propionate Propanoic acid, 3-(carbomethoxymethylthio)-, methyl ester Propanoic acid, 3-(((methoxycarbonyl)methyl)thio)-, methyl ester methyl 3-[(2-methoxy-2-oxoethyl)thio]propionate
Inchi:	InChI=1S/C7H12O4S/c1-10-6(8)3-4-12-5-7(9)11-2/h3-5H2,1-2H3
InchiKey:	XNDKLLFGXIEGKL-UHFFFAOYSA-N
Formula:	C7H12O4S
SMILES:	COC(=O)CCSCC(=O)OC
Mol. weight [g/mol]:	192.23
CAS:	7400-45-5

Physical Properties

Property code	Value	Unit	Source
gf	-426.66	kJ/mol	Joback Method
hf	-635.54	kJ/mol	Joback Method
hfus	23.59	kJ/mol	Joback Method
hvap	56.31	kJ/mol	Joback Method
log10ws	-0.36		Crippen Method
logp	0.456		Crippen Method
mcvol	140.720	ml/mol	McGowan Method
pc	3152.62	kPa	Joback Method
tb	580.92	K	Joback Method
tc	784.42	K	Joback Method
tf	347.37	K	Joback Method
vc	0.529	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	325.49	J/mol×K	580.92	Joback Method
cpg	336.44	J/mol×K	614.84	Joback Method
cpg	346.91	J/mol×K	648.75	Joback Method
cpg	356.88	J/mol×K	682.67	Joback Method

cpg	366.32	J/mol×K	716.58	Joback Method
cpg	375.21	J/mol×K	750.50	Joback Method
cpg	383.55	J/mol×K	784.42	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	414.50 ± 0.50	K	1.70	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7400455&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
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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