3-Thiophenemalonic acid, tetrahydro-, 1,1-dioxide, diethyl ester

Inchi: InChI=1S/C11H18O6S/c1-3-16-10(12)9(11(13)17-4-2)8-5-6-18(14,15)7-8/h8-9H,3-7H2,1

InchiKey: ZRZIZOUPRLJLLK-UHFFFAOYSA-N

Formula: C11H18O6S

SMILES: CCOC(=O)C(C(=O)OCC)C1CCS(=O)(=O)C1

Mol. weight [g/mol]: 278.32

CAS: 4785-62-0

Physical Properties

Property code	Value	Unit	Source
gf	-853.79	kJ/mol	Joback Method
hf	-1154.73	kJ/mol	Joback Method
hfus	31.14	kJ/mol	Joback Method
hvap	75.89	kJ/mol	Joback Method
log10ws	-0.40		Crippen Method
logp	0.163		Crippen Method
mcvol	197.960	ml/mol	McGowan Method
pc	2884.30	kPa	Joback Method
tb	645.33	K	Joback Method
tc	838.78	K	Joback Method
tf	441.56	K	Joback Method
vc	0.752	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	532.71	J/mol×K	645.33	Joback Method
cpg	548.26	J/mol×K	677.57	Joback Method
cpg	562.91	J/mol×K	709.81	Joback Method
cpg	576.67	J/mol×K	742.05	Joback Method
cpg	589.54	J/mol×K	774.30	Joback Method
cpg	601.51	J/mol×K	806.54	Joback Method
cpg	612.60	J/mol×K	838.78	Joback Method

Sources

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=C4785620&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume