Succinic acid, ethyl 4-methylthiophenyl ester

Inchi: InChI=1S/C13H16O4S/c1-3-16-12(14)8-9-13(15)17-10-4-6-11(18-2)7-5-10/h4-7H,3,8-9H
InchiKey: TYJIAACQOQHVNH-UHFFFAOYSA-N
Formula: C13H16O4S
SMILES: CCOC(=O)CCC(=O)Oc1ccc(SC)cc1
Mol. weight [g/mol]: 268.33

Physical Properties

Property code	Value	Unit	Source
gf	-273.36	kJ/mol	Joback Method
hf	-534.32	kJ/mol	Joback Method
hfus	32.78	kJ/mol	Joback Method
hvap	72.60	kJ/mol	Joback Method
log10ws	-3.07		Crippen Method
logp	2.657		Crippen Method
mcvol	201.500	ml/mol	McGowan Method
pc	2400.57	kPa	Joback Method
rinpol	2103.00		NIST Webbook
rinpol	2103.00		NIST Webbook
tb	749.86	K	Joback Method
tc	972.95	K	Joback Method
tf	453.93	K	Joback Method
vc	0.757	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	540.61	J/mol×K	749.86	Joback Method
cpg	553.91	J/mol×K	787.04	Joback Method
cpg	566.18	J/mol×K	824.22	Joback Method
cpg	577.42	J/mol×K	861.40	Joback Method
cpg	587.60	J/mol×K	898.58	Joback Method
cpg	596.75	J/mol×K	935.77	Joback Method
cpg	604.84	J/mol×K	972.95	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U380905&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

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