Succinic acid, di(4-methylthiophenyl) ester

Inchi: InChI=1S/C18H18O4S2/c1-23-15-7-3-13(4-8-15)21-17(19)11-12-18(20)22-14-5-9-16(24-

InchiKey: NJPWAHMYTFAMHX-UHFFFAOYSA-N

Formula: C18H18O4S2

SMILES: CSc1ccc(OC(=O)CCC(=O)Oc2ccc(SC)cc2)cc1

Mol. weight [g/mol]: 362.46

Physical Properties

Property code	Value	Unit	Source
gf	-95.36	kJ/mol	Joback Method
hf	-370.59	kJ/mol	Joback Method
hfus	43.51	kJ/mol	Joback Method
hvap	93.48	kJ/mol	Joback Method
log10ws	-5.24		Crippen Method
logp	4.422		Crippen Method
mcvol	264.540	ml/mol	McGowan Method
pc	2088.84	kPa	Joback Method
rinpol	3126.00		NIST Webbook
rinpol	3126.00		NIST Webbook
tb	964.70	K	Joback Method
tc	1219.43	K	Joback Method
tf	583.62	K	Joback Method
vc	0.984	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	764.70	J/mol×K	964.70	Joback Method
cpg	774.60	J/mol×K	1007.15	Joback Method
cpg	782.76	J/mol×K	1049.61	Joback Method
cpg	789.21	J/mol×K	1092.06	Joback Method
cpg	793.95	J/mol×K	1134.52	Joback Method
cpg	796.99	J/mol×K	1176.97	Joback Method
cpg	798.34	J/mol×K	1219.43	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U380922&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