Succinic acid, 2-methylhex-3-yl 4-methylthiophenyl ester

Inchi: InChI=1S/C18H26O4S/c1-5-6-16(13(2)3)22-18(20)12-11-17(19)21-14-7-9-15(23-4)10-8-1

InchiKey: RXLVZHZTYHAXSP-UHFFFAOYSA-N

Formula: C18H26O4S

SMILES: CCCC(OC(=O)CCC(=O)Oc1ccc(SC)cc1)C(C)C

Mol. weight [g/mol]: 338.46

Physical Properties

Property code	Value	Unit	Source
gf	-236.14	kJ/mol	Joback Method
hf	-648.08	kJ/mol	Joback Method
hfus	38.69	kJ/mol	Joback Method
hvap	82.95	kJ/mol	Joback Method
log10ws	-5.03		Crippen Method
logp	4.462		Crippen Method
mcvol	271.950	ml/mol	McGowan Method
pc	1593.62	kPa	Joback Method
rinpol	2456.00		NIST Webbook
rinpol	2456.00		NIST Webbook
tb	863.38	K	Joback Method
tc	1081.07	K	Joback Method
tf	480.28	K	Joback Method
vc	1.026	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	820.53	J/mol×K	863.38	Joback Method
cpg	835.23	J/mol×K	899.66	Joback Method
cpg	848.62	J/mol×K	935.94	Joback Method
cpg	860.72	J/mol×K	972.22	Joback Method
cpg	871.52	J/mol×K	1008.51	Joback Method
cpg	881.06	J/mol×K	1044.79	Joback Method
cpg	889.33	J/mol×K	1081.07	Joback Method

Sources

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=U380909&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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