Succinic acid, 4-methylthiophenyl octadecyl ester

Inchi: InChI=1S/C29H48O4S/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-25-32-28(30)23-24

InchiKey: RUKQZVNILOQHTD-UHFFFAOYSA-N

Formula: C29H48O4S

SMILES: CCCCCCCCCCCCCCCCCCOC(=O)CCC(=O)Oc1ccc(SC)cc1

Mol. weight [g/mol]: 492.75

Physical Properties

Property code	Value	Unit	Source
gf	-138.64	kJ/mol	Joback Method
hf	-864.56	kJ/mol	Joback Method
hfus	74.22	kJ/mol	Joback Method
hvap	108.22	kJ/mol	Joback Method
log10ws	-9.76		Crippen Method
logp	8.899		Crippen Method
mcvol	426.940	ml/mol	McGowan Method
pc	781.56	kPa	Joback Method
rinpol	3707.00		NIST Webbook
rinpol	3707.00		NIST Webbook
tb	1115.94	K	Joback Method
tc	1379.21	K	Joback Method
tf	634.25	K	Joback Method
vc	1.653	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1488.50	J/mol×K	1115.94	Joback Method
cpg	1504.12	J/mol×K	1159.82	Joback Method
cpg	1517.45	J/mol×K	1203.70	Joback Method
cpg	1528.58	J/mol×K	1247.58	Joback Method
cpg	1537.60	J/mol×K	1291.45	Joback Method
cpg	1544.60	J/mol×K	1335.33	Joback Method
cpg	1549.68	J/mol×K	1379.21	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=U380921&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