Succinic acid, 4-methylthiophenyl pentadecyl ester

Inchi: InChI=1S/C26H42O4S/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-22-29-25(27)20-21-26(28)30

InchiKey: ZTXAYFAONZHYFP-UHFFFAOYSA-N

Formula: C26H42O4S

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

Mol. weight [g/mol]: 450.67

Physical Properties

Property code	Value	Unit	Source
gf	-163.90	kJ/mol	Joback Method
hf	-802.64	kJ/mol	Joback Method
hfus	66.45	kJ/mol	Joback Method
hvap	101.54	kJ/mol	Joback Method
log10ws	-8.51		Crippen Method
logp	7.729		Crippen Method
mcvol	384.670	ml/mol	McGowan Method
pc	924.43	kPa	Joback Method
rinpol	3408.00		NIST Webbook
rinpol	3408.00		NIST Webbook
tb	1047.30	K	Joback Method
tc	1283.70	K	Joback Method
tf	600.44	K	Joback Method
vc	1.486	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1301.49	J/mol×K	1047.30	Joback Method
cpg	1316.70	J/mol×K	1086.70	Joback Method
cpg	1330.08	J/mol×K	1126.10	Joback Method
cpg	1341.70	J/mol×K	1165.50	Joback Method
cpg	1351.59	J/mol×K	1204.90	Joback Method
cpg	1359.82	J/mol×K	1244.30	Joback Method
cpg	1366.44	J/mol×K	1283.70	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U380918&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