Succinic acid, 4-methylthiophenyl tetradecyl ester

Inchi: InChI=1S/C25H40O4S/c1-3-4-5-6-7-8-9-10-11-12-13-14-21-28-24(26)19-20-25(27)29-22

InchiKey: YLMLPGHIXRIQCX-UHFFFAOYSA-N

Formula: C25H40O4S

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

Mol. weight [g/mol]: 436.65

Physical Properties

Property code	Value	Unit	Source
gf	-172.32	kJ/mol	Joback Method
hf	-782.00	kJ/mol	Joback Method
hfus	63.86	kJ/mol	Joback Method
hvap	99.31	kJ/mol	Joback Method
log10ws	-8.09		Crippen Method
logp	7.338		Crippen Method
mcvol	370.580	ml/mol	McGowan Method
pc	980.85	kPa	Joback Method
rinpol	3304.00		NIST Webbook
rinpol	3304.00		NIST Webbook
tb	1024.42	K	Joback Method
tc	1254.40	K	Joback Method
tf	589.17	K	Joback Method
vc	1.429	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1239.69	J/mol×K	1024.42	Joback Method
cpg	1254.78	J/mol×K	1062.75	Joback Method
cpg	1268.17	J/mol×K	1101.08	Joback Method
cpg	1279.89	J/mol×K	1139.41	Joback Method
cpg	1289.99	J/mol×K	1177.74	Joback Method
cpg	1298.52	J/mol×K	1216.07	Joback Method
cpg	1305.52	J/mol×K	1254.40	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U380917&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