Succinic acid, heptadecyl 4-methylthiophenyl ester

Inchi: InChI=1S/C28H46O4S/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-24-31-27(29)22-23-28
InchiKey: OLTAASJSVOGYAO-UHFFFAOYSA-N
Formula: C28H46O4S
SMILES: CCCCCCCCCCCCCCCCCCOC(=O)CCC(=O)Oc1ccc(SC)cc1
Mol. weight [g/mol]: 478.73

Physical Properties

Property code	Value	Unit	Source
gf	-147.06	kJ/mol	Joback Method
hf	-843.92	kJ/mol	Joback Method
hfus	71.63	kJ/mol	Joback Method
hvap	105.99	kJ/mol	Joback Method
log10ws	-9.34		Crippen Method
logp	8.509		Crippen Method
mcvol	412.850	ml/mol	McGowan Method
pc	825.26	kPa	Joback Method
rinpol	3610.00		NIST Webbook
rinpol	3610.00		NIST Webbook
tb	1093.06	K	Joback Method
tc	1346.01	K	Joback Method
tf	622.98	K	Joback Method
vc	1.597	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1425.94	J/mol×K	1093.06	Joback Method
cpg	1441.41	J/mol×K	1135.22	Joback Method
cpg	1454.77	J/mol×K	1177.38	Joback Method
cpg	1466.09	J/mol×K	1219.54	Joback Method
cpg	1475.45	J/mol×K	1261.69	Joback Method
cpg	1482.92	J/mol×K	1303.85	Joback Method
cpg	1488.59	J/mol×K	1346.01	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U380920&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