Succinic acid, decyl 4-methylthiophenyl ester

Inchi: InChI=1S/C21H32O4S/c1-3-4-5-6-7-8-9-10-17-24-20(22)15-16-21(23)25-18-11-13-19(26
InchiKey: SHVMFAWGYSCXMO-UHFFFAOYSA-N
Formula: C21H32O4S
SMILES: CCCCCCCCCCOC(=O)CCC(=O)Oc1ccc(SC)cc1
Mol. weight [g/mol]: 380.54

Physical Properties

Property code	Value	Unit	Source
gf	-206.00	kJ/mol	Joback Method
hf	-699.44	kJ/mol	Joback Method
hfus	53.50	kJ/mol	Joback Method
hvap	90.41	kJ/mol	Joback Method
log10ws	-6.41		Crippen Method
logp	5.778		Crippen Method
mcvol	314.220	ml/mol	McGowan Method
pc	1267.35	kPa	Joback Method
rinpol	2909.00		NIST Webbook
rinpol	2909.00		NIST Webbook
tb	932.90	K	Joback Method
tc	1147.80	K	Joback Method
tf	544.09	K	Joback Method
vc	1.206	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	996.35	J/mol×K	932.90	Joback Method
cpg	1011.07	J/mol×K	968.72	Joback Method
cpg	1024.41	J/mol×K	1004.53	Joback Method
cpg	1036.39	J/mol×K	1040.35	Joback Method
cpg	1047.04	J/mol×K	1076.17	Joback Method
cpg	1056.37	J/mol×K	1111.98	Joback Method
cpg	1064.41	J/mol×K	1147.80	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U380914&Units=SI

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