Succinic acid, hexyl 4-methylthiophenyl ester

Inchi: InChI=1S/C17H24O4S/c1-3-4-5-6-13-20-16(18)11-12-17(19)21-14-7-9-15(22-2)10-8-14/h
InchiKey: XOGWYJSAKKRQAF-UHFFFAOYSA-N
Formula: C17H24O4S
SMILES: CCCCCCOC(=O)CCC(=O)Oc1ccc(SC)cc1
Mol. weight [g/mol]: 324.44

Physical Properties

Property code	Value	Unit	Source
gf	-239.68	kJ/mol	Joback Method
hf	-616.88	kJ/mol	Joback Method
hfus	43.14	kJ/mol	Joback Method
hvap	81.50	kJ/mol	Joback Method
log10ws	-4.74		Crippen Method
logp	4.218		Crippen Method
mcvol	257.860	ml/mol	McGowan Method
pc	1700.50	kPa	Joback Method
rinpol	2498.00		NIST Webbook
rinpol	2498.00		NIST Webbook
tb	841.38	K	Joback Method
tc	1055.08	K	Joback Method
tf	499.01	K	Joback Method
vc	0.982	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	761.89	J/mol×K	841.38	Joback Method
cpg	776.18	J/mol×K	877.00	Joback Method
cpg	789.28	J/mol×K	912.61	Joback Method
cpg	801.20	J/mol×K	948.23	Joback Method
cpg	811.95	J/mol×K	983.85	Joback Method
cpg	821.53	J/mol×K	1019.46	Joback Method
cpg	829.96	J/mol×K	1055.08	Joback Method

Sources

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=U380910&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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