Succinic acid, 4-methylthiophenyl pentyl ester

Inchi: InChI=1S/C16H22O4S/c1-3-4-5-12-19-15(17)10-11-16(18)20-13-6-8-14(21-2)9-7-13/h6-9
InchiKey: ZUCNASGCTWDBLR-UHFFFAOYSA-N
Formula: C16H22O4S
SMILES: CCCCCOC(=O)CCC(=O)Oc1ccc(SC)cc1
Mol. weight [g/mol]: 310.41

Physical Properties

Property code	Value	Unit	Source
gf	-248.10	kJ/mol	Joback Method
hf	-596.24	kJ/mol	Joback Method
hfus	40.55	kJ/mol	Joback Method
hvap	79.28	kJ/mol	Joback Method
log10ws	-4.32		Crippen Method
logp	3.828		Crippen Method
mcvol	243.770	ml/mol	McGowan Method
pc	1843.58	kPa	Joback Method
rinpol	2398.00		NIST Webbook
rinpol	2398.00		NIST Webbook
tb	818.50	K	Joback Method
tc	1033.67	K	Joback Method
tf	487.74	K	Joback Method
vc	0.925	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	705.15	J/mol×K	818.50	Joback Method
cpg	719.27	J/mol×K	854.36	Joback Method
cpg	732.24	J/mol×K	890.22	Joback Method
cpg	744.06	J/mol×K	926.08	Joback Method
cpg	754.75	J/mol×K	961.94	Joback Method
cpg	764.30	J/mol×K	997.80	Joback Method
cpg	772.72	J/mol×K	1033.67	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=U380908&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