Succinic acid, hexadecyl 4-methylthiophenyl ester

Inchi: InChI=1S/C27H44O4S/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-23-30-26(28)21-22-27(29

InchiKey: PRJIXIKNYXIIGX-UHFFFAOYSA-N

Formula: C27H44O4S

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

Mol. weight [g/mol]: 464.70

Physical Properties

Property code	Value	Unit	Source
gf	-155.48	kJ/mol	Joback Method
hf	-823.28	kJ/mol	Joback Method
hfus	69.04	kJ/mol	Joback Method
hvap	103.76	kJ/mol	Joback Method
log10ws	-8.93		Crippen Method
logp	8.119		Crippen Method
mcvol	398.760	ml/mol	McGowan Method
pc	872.74	kPa	Joback Method
rinpol	3507.00		NIST Webbook
rinpol	3507.00		NIST Webbook
tb	1070.18	K	Joback Method
tc	1314.21	K	Joback Method
tf	611.71	K	Joback Method
vc	1.542	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1363.59	J/mol×K	1070.18	Joback Method
cpg	1378.92	J/mol×K	1110.85	Joback Method
cpg	1392.30	J/mol×K	1151.52	Joback Method
cpg	1403.78	J/mol×K	1192.19	Joback Method
cpg	1413.43	J/mol×K	1232.86	Joback Method
cpg	1421.31	J/mol×K	1273.54	Joback Method
cpg	1427.48	J/mol×K	1314.21	Joback Method

Sources

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=U380919&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

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