Diethylmalonic acid, 2-methylthiophenyl tridecyl ester

Inchi: InChI=1S/C27H44O4S/c1-5-8-9-10-11-12-13-14-15-16-19-22-30-25(28)27(6-2,7-3)26(29
InchiKey: CSEQVDFPTDFLOA-UHFFFAOYSA-N
Formula: C27H44O4S
SMILES: CCCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)Oc1ccccc1SC
Mol. weight [g/mol]: 464.70

Physical Properties

Property code	Value	Unit	Source
gf	-152.64	kJ/mol	Joback Method
hf	-832.03	kJ/mol	Joback Method
hfus	61.63	kJ/mol	Joback Method
hvap	102.47	kJ/mol	Joback Method
log10ws	-8.68		Crippen Method
logp	7.974		Crippen Method
mcvol	398.760	ml/mol	McGowan Method
pc	882.62	kPa	Joback Method
rinpol	3170.00		NIST Webbook
tb	1066.95	K	Joback Method
tc	1307.51	K	Joback Method
tf	614.13	K	Joback Method
vc	1.530	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1363.83	J/mol×K	1066.95	Joback Method
cpg	1379.41	J/mol×K	1107.04	Joback Method
cpg	1393.29	J/mol×K	1147.14	Joback Method
cpg	1405.57	J/mol×K	1187.23	Joback Method
cpg	1416.33	J/mol×K	1227.32	Joback Method
cpg	1425.67	J/mol×K	1267.42	Joback Method
cpg	1433.66	J/mol×K	1307.51	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U369539&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

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