Diethylmalonic acid, dodecyl 2-methylthiophenyl ester

Inchi: InChI=1S/C26H42O4S/c1-5-8-9-10-11-12-13-14-15-18-21-29-24(27)26(6-2,7-3)25(28)30
InchiKey: UOSNZMOAEZPPFA-UHFFFAOYSA-N
Formula: C26H42O4S
SMILES: CCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)Oc1ccccc1SC
Mol. weight [g/mol]: 450.67

Physical Properties

Property code	Value	Unit	Source
gf	-161.06	kJ/mol	Joback Method
hf	-811.39	kJ/mol	Joback Method
hfus	59.04	kJ/mol	Joback Method
hvap	100.24	kJ/mol	Joback Method
log10ws	-8.27		Crippen Method
logp	7.584		Crippen Method
mcvol	384.670	ml/mol	McGowan Method
pc	935.20	kPa	Joback Method
rinpol	3065.00		NIST Webbook
rinpol	3065.00		NIST Webbook
tb	1044.07	K	Joback Method
tc	1278.37	K	Joback Method
tf	602.86	K	Joback Method
vc	1.474	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1301.63	J/mol×K	1044.07	Joback Method
cpg	1317.04	J/mol×K	1083.12	Joback Method
cpg	1330.83	J/mol×K	1122.17	Joback Method
cpg	1343.10	J/mol×K	1161.22	Joback Method
cpg	1353.91	J/mol×K	1200.27	Joback Method
cpg	1363.35	J/mol×K	1239.32	Joback Method
cpg	1371.48	J/mol×K	1278.37	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U369538&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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