Diethylmalonic acid, 2-methylthiophenyl tetradecyl ester

Inchi: InChI=1S/C28H46O4S/c1-5-8-9-10-11-12-13-14-15-16-17-20-23-31-26(29)28(6-2,7-3)27

InchiKey: URIPXTJCBXXHIH-UHFFFAOYSA-N

Formula: C28H46O4S

SMILES: CCCCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)Oc1ccccc1SC

Mol. weight [g/mol]: 478.73

Physical Properties

Property code	Value	Unit	Source
gf	-144.22	kJ/mol	Joback Method
hf	-852.67	kJ/mol	Joback Method
hfus	64.22	kJ/mol	Joback Method
hvap	104.69	kJ/mol	Joback Method
log10ws	-9.10		Crippen Method
logp	8.365		Crippen Method
mcvol	412.850	ml/mol	McGowan Method
pc	834.35	kPa	Joback Method
rinpol	3273.00		NIST Webbook
tb	1089.83	K	Joback Method
tc	1337.88	K	Joback Method
tf	625.40	K	Joback Method
vc	1.587	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1426.35	J/mol×K	1089.83	Joback Method
cpg	1442.13	J/mol×K	1131.17	Joback Method
cpg	1456.12	J/mol×K	1172.51	Joback Method
cpg	1468.42	J/mol×K	1213.85	Joback Method
cpg	1479.13	J/mol×K	1255.19	Joback Method
cpg	1488.35	J/mol×K	1296.53	Joback Method
cpg	1496.19	J/mol×K	1337.88	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=U369540&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