Diethylmalonic acid, 2-methylthiophenyl pentadecyl ester

Inchi: InChI=1S/C29H48O4S/c1-5-8-9-10-11-12-13-14-15-16-17-18-21-24-32-27(30)29(6-2,7-3
InchiKey: MYAQQTCWJAFKST-UHFFFAOYSA-N
Formula: C29H48O4S
SMILES: CCCCCCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)Oc1ccccc1SC
Mol. weight [g/mol]: 492.75

Physical Properties

Property code	Value	Unit	Source
gf	-135.80	kJ/mol	Joback Method
hf	-873.31	kJ/mol	Joback Method
hfus	66.81	kJ/mol	Joback Method
hvap	106.92	kJ/mol	Joback Method
log10ws	-9.52		Crippen Method
logp	8.755		Crippen Method
mcvol	426.940	ml/mol	McGowan Method
pc	789.93	kPa	Joback Method
rinpol	3395.00		NIST Webbook
rinpol	3395.00		NIST Webbook
tb	1112.71	K	Joback Method
tc	1369.55	K	Joback Method
tf	636.67	K	Joback Method
vc	1.643	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1489.15	J/mol×K	1112.71	Joback Method
cpg	1505.17	J/mol×K	1155.52	Joback Method
cpg	1519.28	J/mol×K	1198.32	Joback Method
cpg	1531.61	J/mol×K	1241.13	Joback Method
cpg	1542.26	J/mol×K	1283.94	Joback Method
cpg	1551.37	J/mol×K	1326.74	Joback Method
cpg	1559.05	J/mol×K	1369.55	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=U369541&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