Diethylmalonic acid, hexadecyl 2-methylthiophenyl ester

Inchi: InChI=1S/C30H50O4S/c1-5-8-9-10-11-12-13-14-15-16-17-18-19-22-25-33-28(31)30(6-2,
InchiKey: JZSYIMPVWQQFOX-UHFFFAOYSA-N
Formula: C30H50O4S
SMILES: CCCCCCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)Oc1ccccc1SC
Mol. weight [g/mol]: 506.78

Physical Properties

Property code	Value	Unit	Source
gf	-127.38	kJ/mol	Joback Method
hf	-893.95	kJ/mol	Joback Method
hfus	69.40	kJ/mol	Joback Method
hvap	109.15	kJ/mol	Joback Method
log10ws	-9.94		Crippen Method
logp	9.145		Crippen Method
mcvol	441.030	ml/mol	McGowan Method
pc	748.97	kPa	Joback Method
rinpol	3549.00		NIST Webbook
rinpol	3549.00		NIST Webbook
tb	1135.59	K	Joback Method
tc	1402.63	K	Joback Method
tf	647.94	K	Joback Method
vc	1.698	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1552.20	J/mol×K	1135.59	Joback Method
cpg	1568.49	J/mol×K	1180.10	Joback Method
cpg	1582.75	J/mol×K	1224.60	Joback Method
cpg	1595.12	J/mol×K	1269.11	Joback Method
cpg	1605.72	J/mol×K	1313.62	Joback Method
cpg	1614.72	J/mol×K	1358.12	Joback Method
cpg	1622.23	J/mol×K	1402.63	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U369542&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