Diethylmalonic acid, decyl 2-methylthiophenyl ester

Inchi: InChI=1S/C24H38O4S/c1-5-8-9-10-11-12-13-16-19-27-22(25)24(6-2,7-3)23(26)28-20-17

InchiKey: YWDROAFFNSVCQP-UHFFFAOYSA-N

Formula: C24H38O4S

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

Mol. weight [g/mol]: 422.62

Physical Properties

Property code	Value	Unit	Source
gf	-177.90	kJ/mol	Joback Method
hf	-770.11	kJ/mol	Joback Method
hfus	53.86	kJ/mol	Joback Method
hvap	95.79	kJ/mol	Joback Method
log10ws	-7.43		Crippen Method
logp	6.804		Crippen Method
mcvol	356.490	ml/mol	McGowan Method
pc	1055.51	kPa	Joback Method
rinpol	2861.00		NIST Webbook
tb	998.31	K	Joback Method
tc	1223.44	K	Joback Method
tf	580.32	K	Joback Method
vc	1.363	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1178.33	J/mol×K	998.31	Joback Method
cpg	1193.47	J/mol×K	1035.83	Joback Method
cpg	1207.13	J/mol×K	1073.35	Joback Method
cpg	1219.39	J/mol×K	1110.87	Joback Method
cpg	1230.30	J/mol×K	1148.39	Joback Method
cpg	1239.91	J/mol×K	1185.92	Joback Method
cpg	1248.30	J/mol×K	1223.44	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U369537&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