Diethylmalonic acid, di(2-methylthiophenyl) ester

Inchi: InChI=1S/C21H24O4S2/c1-5-21(6-2,19(22)24-15-11-7-9-13-17(15)26-3)20(23)25-16-12-

InchiKey: ZYKIUWUJXHNJIR-UHFFFAOYSA-N

Formula: C21H24O4S2

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

Mol. weight [g/mol]: 404.54

Physical Properties

Property code	Value	Unit	Source
gf	-67.26	kJ/mol	Joback Method
hf	-441.26	kJ/mol	Joback Method
hfus	43.87	kJ/mol	Joback Method
hvap	98.87	kJ/mol	Joback Method
log10ws	-6.25		Crippen Method
logp	5.448		Crippen Method
mcvol	306.810	ml/mol	McGowan Method
pc	1656.49	kPa	Joback Method
rinpol	2971.00		NIST Webbook
tb	1030.11	K	Joback Method
tc	1285.90	K	Joback Method
tf	619.85	K	Joback Method
vc	1.141	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	937.38	J/mol×K	1030.11	Joback Method
cpg	947.34	J/mol×K	1072.74	Joback Method
cpg	955.61	J/mol×K	1115.37	Joback Method
cpg	962.26	J/mol×K	1158.00	Joback Method
cpg	967.34	J/mol×K	1200.64	Joback Method
cpg	970.91	J/mol×K	1243.27	Joback Method
cpg	973.04	J/mol×K	1285.90	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U369543&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

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