Diethylmalonic acid, butyl 2-methylthiophenyl ester

Inchi: InChI=1S/C18H26O4S/c1-5-8-13-21-16(19)18(6-2,7-3)17(20)22-14-11-9-10-12-15(14)23

InchiKey: YEXOVYVKSIKZHJ-UHFFFAOYSA-N

Formula: C18H26O4S

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

Mol. weight [g/mol]: 338.46

Physical Properties

Property code	Value	Unit	Source
gf	-228.42	kJ/mol	Joback Method
hf	-646.27	kJ/mol	Joback Method
hfus	38.32	kJ/mol	Joback Method
hvap	82.43	kJ/mol	Joback Method
log10ws	-4.92		Crippen Method
logp	4.464		Crippen Method
mcvol	271.950	ml/mol	McGowan Method
pc	1597.44	kPa	Joback Method
rinpol	2275.00		NIST Webbook
tb	861.03	K	Joback Method
tc	1080.82	K	Joback Method
tf	512.70	K	Joback Method
vc	1.026	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	820.49	J/mol×K	861.03	Joback Method
cpg	835.13	J/mol×K	897.66	Joback Method
cpg	848.52	J/mol×K	934.29	Joback Method
cpg	860.68	J/mol×K	970.93	Joback Method
cpg	871.67	J/mol×K	1007.56	Joback Method
cpg	881.50	J/mol×K	1044.19	Joback Method
cpg	890.21	J/mol×K	1080.82	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=U369531&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