Terephthalic acid, 4-methylthiophenyl propyl ester

Inchi: InChI=1S/C18H18O4S/c1-3-12-21-17(19)13-4-6-14(7-5-13)18(20)22-15-8-10-16(23-2)11

InchiKey: VPHUHSWTHPBCSS-UHFFFAOYSA-N

Formula: C18H18O4S

SMILES: CCCOC(=O)c1ccc(C(=O)Oc2ccc(SC)cc2)cc1

Mol. weight [g/mol]: 330.40

Physical Properties

Property code	Value	Unit	Source
gf	-128.48	kJ/mol	Joback Method
hf	-412.46	kJ/mol	Joback Method
hfus	39.38	kJ/mol	Joback Method
hvap	86.67	kJ/mol	Joback Method
log10ws	-5.38		Crippen Method
logp	4.194		Crippen Method
mcvol	248.190	ml/mol	McGowan Method
pc	2056.76	kPa	Joback Method
rinpol	2858.00		NIST Webbook
rinpol	2858.00		NIST Webbook
tb	895.92	K	Joback Method
tc	1138.18	K	Joback Method
tf	549.22	K	Joback Method
vc	0.929	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	717.99	J/mol×K	895.92	Joback Method
cpg	730.18	J/mol×K	936.30	Joback Method
cpg	740.92	J/mol×K	976.67	Joback Method
cpg	750.21	J/mol×K	1017.05	Joback Method
cpg	758.10	J/mol×K	1057.42	Joback Method
cpg	764.58	J/mol×K	1097.80	Joback Method
cpg	769.68	J/mol×K	1138.18	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U416119&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

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