Phthalic acid, ethyl 2-(methylthio)phenyl ester

Inchi: InChI=1S/C17H16O4S/c1-3-20-16(18)12-8-4-5-9-13(12)17(19)21-14-10-6-7-11-15(14)22
InchiKey: XJYXXBRNDRZRDD-UHFFFAOYSA-N
Formula: C17H16O4S
SMILES: CCOC(=O)c1ccccc1C(=O)Oc1ccccc1SC
Mol. weight [g/mol]: 316.37

Physical Properties

Property code	Value	Unit	Source
gf	-136.90	kJ/mol	Joback Method
hf	-391.82	kJ/mol	Joback Method
hfus	36.79	kJ/mol	Joback Method
hvap	84.44	kJ/mol	Joback Method
log10ws	-4.96		Crippen Method
logp	3.804		Crippen Method
mcvol	234.100	ml/mol	McGowan Method
pc	2248.26	kPa	Joback Method
rinpol	2575.00		NIST Webbook
rinpol	2575.00		NIST Webbook
tb	873.04	K	Joback Method
tc	1118.87	K	Joback Method
tf	537.95	K	Joback Method
vc	0.874	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	661.94	J/mol×K	873.04	Joback Method
cpg	674.07	J/mol×K	914.01	Joback Method
cpg	684.76	J/mol×K	954.98	Joback Method
cpg	694.03	J/mol×K	995.96	Joback Method
cpg	701.90	J/mol×K	1036.93	Joback Method
cpg	708.37	J/mol×K	1077.90	Joback Method
cpg	713.46	J/mol×K	1118.87	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=U415558&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