Phthalic acid, di(2-(methylthio)phenyl) ester

Inchi: InChI=1S/C22H18O4S2/c1-27-19-13-7-5-11-17(19)25-21(23)15-9-3-4-10-16(15)22(24)26
InchiKey: TZYPGJFJFHIKOH-UHFFFAOYSA-N
Formula: C22H18O4S2
SMILES: CSc1ccccc1OC(=O)c1ccccc1C(=O)Oc1ccccc1SC
Mol. weight [g/mol]: 410.51

Physical Properties

Property code	Value	Unit	Source
gf	41.10	kJ/mol	Joback Method
hf	-228.09	kJ/mol	Joback Method
hfus	47.53	kJ/mol	Joback Method
hvap	105.33	kJ/mol	Joback Method
log10ws	-7.13		Crippen Method
logp	5.569		Crippen Method
mcvol	297.140	ml/mol	McGowan Method
pc	1964.82	kPa	Joback Method
rinpol	1510.00		NIST Webbook
rinpol	1510.00		NIST Webbook
tb	1087.88	K	Joback Method
tc	1363.05	K	Joback Method
tf	667.64	K	Joback Method
vc	1.099	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	875.19	J/mol×K	1087.88	Joback Method
cpg	881.16	J/mol×K	1133.74	Joback Method
cpg	885.08	J/mol×K	1179.60	Joback Method
cpg	886.97	J/mol×K	1225.47	Joback Method
cpg	886.89	J/mol×K	1271.33	Joback Method
cpg	884.87	J/mol×K	1317.19	Joback Method
cpg	880.96	J/mol×K	1363.05	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=U415565&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