Phthalic acid, isobutyl 2-(methylthio)phenyl ester

Inchi: InChI=1S/C19H20O4S/c1-13(2)12-22-18(20)14-8-4-5-9-15(14)19(21)23-16-10-6-7-11-17

InchiKey: DDZKFPIKKWYWSZ-UHFFFAOYSA-N

Formula: C19H20O4S

SMILES: CSc1ccccc1OC(=O)c1ccccc1C(=O)OCC(C)C

Mol. weight [g/mol]: 344.43

Physical Properties

Property code	Value	Unit	Source
gf	-122.50	kJ/mol	Joback Method
hf	-438.38	kJ/mol	Joback Method
hfus	38.45	kJ/mol	Joback Method
hvap	88.50	kJ/mol	Joback Method
log10ws	-5.56		Crippen Method
logp	4.440		Crippen Method
mcvol	262.280	ml/mol	McGowan Method
pc	1901.92	kPa	Joback Method
rinpol	2723.00		NIST Webbook
rinpol	2723.00		NIST Webbook
tb	918.36	K	Joback Method
tc	1160.99	K	Joback Method
tf	545.49	K	Joback Method
vc	0.980	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	775.28	J/mol×K	918.36	Joback Method
cpg	787.61	J/mol×K	958.80	Joback Method
cpg	798.40	J/mol×K	999.24	Joback Method
cpg	807.69	J/mol×K	1039.68	Joback Method
cpg	815.49	J/mol×K	1080.11	Joback Method
cpg	821.83	J/mol×K	1120.55	Joback Method
cpg	826.74	J/mol×K	1160.99	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415560&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