Phthalic acid, butyl 2-(methylthio)phenyl ester

Inchi: InChI=1S/C19H20O4S/c1-3-4-13-22-18(20)14-9-5-6-10-15(14)19(21)23-16-11-7-8-12-17
InchiKey: XOTASCIYCMDVMM-UHFFFAOYSA-N
Formula: C19H20O4S
SMILES: CCCCOC(=O)c1ccccc1C(=O)Oc1ccccc1SC
Mol. weight [g/mol]: 344.43

Physical Properties

Property code	Value	Unit	Source
gf	-120.06	kJ/mol	Joback Method
hf	-433.10	kJ/mol	Joback Method
hfus	41.97	kJ/mol	Joback Method
hvap	88.89	kJ/mol	Joback Method
log10ws	-5.80		Crippen Method
logp	4.585		Crippen Method
mcvol	262.280	ml/mol	McGowan Method
pc	1888.72	kPa	Joback Method
rinpol	2820.00		NIST Webbook
rinpol	2820.00		NIST Webbook
tb	918.80	K	Joback Method
tc	1158.19	K	Joback Method
tf	560.49	K	Joback Method
vc	0.986	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	774.76	J/mol×K	918.80	Joback Method
cpg	786.97	J/mol×K	958.70	Joback Method
cpg	797.70	J/mol×K	998.60	Joback Method
cpg	806.98	J/mol×K	1038.50	Joback Method
cpg	814.84	J/mol×K	1078.39	Joback Method
cpg	821.28	J/mol×K	1118.29	Joback Method
cpg	826.34	J/mol×K	1158.19	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415561&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