Phthalic acid, 2-(methylthio)phenyl pentyl ester

Inchi: InChI=1S/C20H22O4S/c1-3-4-9-14-23-19(21)15-10-5-6-11-16(15)20(22)24-17-12-7-8-13

InchiKey: DHBKNWQGPNBFHR-UHFFFAOYSA-N

Formula: C20H22O4S

SMILES: CCCCCOC(=O)c1ccccc1C(=O)Oc1ccccc1SC

Mol. weight [g/mol]: 358.45

Physical Properties

Property code	Value	Unit	Source
gf	-111.64	kJ/mol	Joback Method
hf	-453.74	kJ/mol	Joback Method
hfus	44.56	kJ/mol	Joback Method
hvap	91.12	kJ/mol	Joback Method
log10ws	-6.22		Crippen Method
logp	4.975		Crippen Method
mcvol	276.370	ml/mol	McGowan Method
pc	1740.46	kPa	Joback Method
rinpol	2920.00		NIST Webbook
rinpol	2920.00		NIST Webbook
tb	941.68	K	Joback Method
tc	1178.95	K	Joback Method
tf	571.76	K	Joback Method
vc	1.042	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	832.19	J/mol×K	941.68	Joback Method
cpg	844.38	J/mol×K	981.23	Joback Method
cpg	855.08	J/mol×K	1020.77	Joback Method
cpg	864.30	J/mol×K	1060.32	Joback Method
cpg	872.08	J/mol×K	1099.86	Joback Method
cpg	878.44	J/mol×K	1139.41	Joback Method
cpg	883.42	J/mol×K	1178.95	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=U415562&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

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