Phthalic acid, heptyl 2-(methylthio)phenyl ester

Inchi: InChI=1S/C22H26O4S/c1-3-4-5-6-11-16-25-21(23)17-12-7-8-13-18(17)22(24)26-19-14-9

InchiKey: RZKBBCUMYCJRHB-UHFFFAOYSA-N

Formula: C22H26O4S

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

Mol. weight [g/mol]: 386.50

Physical Properties

Property code	Value	Unit	Source
gf	-94.80	kJ/mol	Joback Method
hf	-495.02	kJ/mol	Joback Method
hfus	49.74	kJ/mol	Joback Method
hvap	95.57	kJ/mol	Joback Method
log10ws	-7.06		Crippen Method
logp	5.755		Crippen Method
mcvol	304.550	ml/mol	McGowan Method
pc	1491.89	kPa	Joback Method
rinpol	1466.00		NIST Webbook
rinpol	1466.00		NIST Webbook
tb	987.44	K	Joback Method
tc	1222.87	K	Joback Method
tf	594.30	K	Joback Method
vc	1.153	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	948.79	J/mol×K	987.44	Joback Method
cpg	960.87	J/mol×K	1026.68	Joback Method
cpg	971.40	J/mol×K	1065.92	Joback Method
cpg	980.42	J/mol×K	1105.16	Joback Method
cpg	987.94	J/mol×K	1144.40	Joback Method
cpg	994.03	J/mol×K	1183.64	Joback Method
cpg	998.69	J/mol×K	1222.87	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415564&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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