3-(Methylthio)benzoic acid, 2,3,4,5-tetrafluorobenzyl ester

Inchi: InChI=1S/C15H10F4O2S/c1-22-10-4-2-3-8(5-10)15(20)21-7-9-6-11(16)13(18)14(19)12(9

InchiKey: DPHMTXCFSOKVEP-UHFFFAOYSA-N

Formula: C15H10F4O2S

SMILES: CSc1cccc(C(=O)OCc2cc(F)c(F)c(F)c2F)c1

Mol. weight [g/mol]: 330.30

Physical Properties

Property code	Value	Unit	Source
gf	-727.95	kJ/mol	Joback Method
hf	-924.59	kJ/mol	Joback Method
hfus	39.98	kJ/mol	Joback Method
hvap	69.55	kJ/mol	Joback Method
log10ws	-5.89		Crippen Method
logp	4.322		Crippen Method
mcvol	205.560	ml/mol	McGowan Method
pc	2088.84	kPa	Joback Method
rinpol	2124.00		NIST Webbook
rinpol	2124.00		NIST Webbook
tb	763.01	K	Joback Method
tc	980.89	K	Joback Method
tf	483.17	K	Joback Method
vc	0.809	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	544.05	J/mol×K	763.01	Joback Method
cpg	555.69	J/mol×K	799.32	Joback Method
cpg	566.40	J/mol×K	835.64	Joback Method
cpg	576.18	J/mol×K	871.95	Joback Method
cpg	585.03	J/mol×K	908.26	Joback Method
cpg	592.97	J/mol×K	944.57	Joback Method
cpg	600.00	J/mol×K	980.89	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U375056&Units=SI

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