3-(Methylthio)benzoic acid, 2-(pentafluorophenoxy)ethyl ester

Inchi: InChI=1S/C16H11F5O3S/c1-25-9-4-2-3-8(7-9)16(22)24-6-5-23-15-13(20)11(18)10(17)12

InchiKey: IBYFVLGCBXUHNB-UHFFFAOYSA-N

Formula: C16H11F5O3S

SMILES: CSc1cccc(C(=O)OCCOc2c(F)c(F)c(F)c(F)c2F)c1

Mol. weight [g/mol]: 378.31

Physical Properties

Property code	Value	Unit	Source
gf	-1028.97	kJ/mol	Joback Method
hf	-1285.03	kJ/mol	Joback Method
hfus	46.45	kJ/mol	Joback Method
hvap	74.03	kJ/mol	Joback Method
log10ws	-5.88		Crippen Method
logp	4.340		Crippen Method
mcvol	227.290	ml/mol	McGowan Method
pc	1793.94	kPa	Joback Method
rinpol	2239.00		NIST Webbook
rinpol	2239.00		NIST Webbook
tb	812.56	K	Joback Method
tc	1020.86	K	Joback Method
tf	529.78	K	Joback Method
vc	0.901	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	629.20	J/mol×K	812.56	Joback Method
cpg	640.30	J/mol×K	847.28	Joback Method
cpg	650.42	J/mol×K	881.99	Joback Method
cpg	659.57	J/mol×K	916.71	Joback Method
cpg	667.72	J/mol×K	951.43	Joback Method
cpg	674.88	J/mol×K	986.14	Joback Method
cpg	681.02	J/mol×K	1020.86	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=U375060&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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