Benzoic acid, 2-(heptafluorobutyrylthio)-, methyl ester

Inchi: InChI=1S/C12H7F7O3S/c1-22-8(20)6-4-2-3-5-7(6)23-9(21)10(13,14)11(15,16)12(17,18)1

InchiKey: WTDRLHGFTIFOMF-UHFFFAOYSA-N

Formula: C12H7F7O3S

SMILES: COC(=O)c1ccccc1SC(=O)C(F)(F)C(F)(F)C(F)(F)F

Mol. weight [g/mol]: 364.24

Physical Properties

Property code	Value	Unit	Source
gf	-1531.93	kJ/mol	Joback Method
hf	-1780.48	kJ/mol	Joback Method
hfus	28.32	kJ/mol	Joback Method
hvap	58.36	kJ/mol	Joback Method
log10ws	-4.78		Crippen Method
logp	3.925		Crippen Method
mcvol	193.930	ml/mol	McGowan Method
pc	2092.66	kPa	Joback Method
rinpol	1432.00		NIST Webbook
rinpol	1432.00		NIST Webbook
tb	689.76	K	Joback Method
tc	890.03	K	Joback Method
tf	431.82	K	Joback Method
vc	0.776	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	527.86	J/mol×K	689.76	Joback Method
cpg	538.14	J/mol×K	723.14	Joback Method
cpg	547.49	J/mol×K	756.52	Joback Method
cpg	555.99	J/mol×K	789.89	Joback Method
cpg	563.69	J/mol×K	823.27	Joback Method
cpg	570.67	J/mol×K	856.65	Joback Method
cpg	576.98	J/mol×K	890.03	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=U375161&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