3-(Methylthio)propyl 2,3,4,5,6-pentafluorobenzoate

Inchi: InChI=1S/C11H9F5O2S/c1-19-4-2-3-18-11(17)5-6(12)8(14)10(16)9(15)7(5)13/h2-4H2,1H

InchiKey: MKSFUAZEEQSRPY-UHFFFAOYSA-N

Formula: C11H9F5O2S

SMILES: CSCCCOC(=O)c1c(F)c(F)c(F)c(F)c1F

Mol. weight [g/mol]: 300.25

Physical Properties

Property code	Value	Unit	Source
gf	-1068.85	kJ/mol	Joback Method
hf	-1274.67	kJ/mol	Joback Method
hfus	38.66	kJ/mol	Joback Method
hvap	57.55	kJ/mol	Joback Method
log10ws	-4.51		Crippen Method
logp	3.292		Crippen Method
mcvol	174.730	ml/mol	McGowan Method
pc	2104.20	kPa	Joback Method
rinpol	1570.00		NIST Webbook
rinpol	1570.00		NIST Webbook
tb	644.08	K	Joback Method
tc	830.74	K	Joback Method
tf	412.26	K	Joback Method
vc	0.712	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	434.92	J/mol×K	644.08	Joback Method
cpg	445.43	J/mol×K	675.19	Joback Method
cpg	455.42	J/mol×K	706.30	Joback Method
cpg	464.87	J/mol×K	737.41	Joback Method
cpg	473.80	J/mol×K	768.52	Joback Method
cpg	482.17	J/mol×K	799.63	Joback Method
cpg	490.00	J/mol×K	830.74	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U378293&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

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