

Benzoic acid, 3-(pentafluoropropionylthio)-

Inchi: InChI=1S/C10H5F5O3S/c11-9(12,10(13,14)15)8(18)19-6-3-1-2-5(4-6)7(16)17/h1-4H,(H,1)
InchiKey: VRTCZLDKAZAKNU-UHFFFAOYSA-N
Formula: C10H5F5O3S
SMILES: O=C(O)c1cccc(SC(=O)C(F)(F)C(F)(F)F)c1
Mol. weight [g/mol]: 300.20

Physical Properties

Property code	Value	Unit	Source
gf	-1193.81	kJ/mol	Joback Method
hf	-1358.24	kJ/mol	Joback Method
hfus	27.30	kJ/mol	Joback Method
hvap	71.10	kJ/mol	Joback Method
log10ws	-3.86		Crippen Method
logp	3.201		Crippen Method
mcvol	162.210	ml/mol	McGowan Method
pc	3038.96	kPa	Joback Method
rinpol	1507.00		NIST Webbook
rinpol	1507.00		NIST Webbook
tb	718.45	K	Joback Method
tc	920.35	K	Joback Method
tf	444.27	K	Joback Method
vc	0.640	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	429.72	J/mol×K	718.45	Joback Method
cpg	437.33	J/mol×K	752.10	Joback Method
cpg	444.22	J/mol×K	785.75	Joback Method
cpg	450.47	J/mol×K	819.40	Joback Method
cpg	456.13	J/mol×K	853.05	Joback Method
cpg	461.25	J/mol×K	886.70	Joback Method
cpg	465.88	J/mol×K	920.35	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=U375173&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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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