Benzoic acid, 3-(heptafluorobutyrylthio)-

Inchi: InChI=1S/C11H5F7O3S/c12-9(13,10(14,15)11(16,17)18)8(21)22-6-3-1-2-5(4-6)7(19)20/h
InchiKey: NERQSFXREBYQNJ-UHFFFAOYSA-N
Formula: C11H5F7O3S
SMILES: O=C(O)c1cccc(SC(=O)C(F)(F)C(F)(F)C(F)(F)F)c1
Mol. weight [g/mol]: 350.21

Physical Properties

Property code	Value	Unit	Source
gf	-1572.17	kJ/mol	Joback Method
hf	-1779.85	kJ/mol	Joback Method
hfus	28.63	kJ/mol	Joback Method
hvap	70.40	kJ/mol	Joback Method
log10ws	-4.60		Crippen Method
logp	3.836		Crippen Method
mcvol	179.840	ml/mol	McGowan Method
pc	2548.19	kPa	Joback Method
rinpol	1543.00		NIST Webbook
tb	736.64	K	Joback Method
tc	931.53	K	Joback Method
tf	459.14	K	Joback Method
vc	0.722	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	498.19	J/mol×K	736.64	Joback Method
cpg	505.68	J/mol×K	769.12	Joback Method
cpg	512.47	J/mol×K	801.60	Joback Method
cpg	518.60	J/mol×K	834.08	Joback Method
cpg	524.16	J/mol×K	866.56	Joback Method
cpg	529.22	J/mol×K	899.04	Joback Method
cpg	533.84	J/mol×K	931.53	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U375171&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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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