Perfluoro-pentan ethioic acid S-butyl ester

Inchi: InChI=1S/C9H9F9OS/c1-2-3-4-20-5(19)6(10,11)7(12,13)8(14,15)9(16,17)18/h2-4H2,1H3
InchiKey: ZYEPLCLZSHCXDZ-UHFFFAOYSA-N
Formula: C9H9F9OS
SMILES: CCCCSC(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 336.22

Physical Properties

Property code	Value	Unit	Source
gf	-1812.83	kJ/mol	Joback Method
hf	-2099.79	kJ/mol	Joback Method
hfus	22.86	kJ/mol	Joback Method
hvap	36.65	kJ/mol	Joback Method
log10ws	-4.85		Crippen Method
logp	4.514		Crippen Method
mcvol	171.520	ml/mol	McGowan Method
pc	1840.41	kPa	Joback Method
rinpol	953.00		NIST Webbook
rinpol	946.00		NIST Webbook
rinpol	946.00		NIST Webbook
rinpol	941.00		NIST Webbook
rinpol	931.00		NIST Webbook
ripol	1008.00		NIST Webbook
ripol	957.00		NIST Webbook
ripol	983.00		NIST Webbook
ripol	945.00		NIST Webbook
ripol	1008.00		NIST Webbook
tb	508.48	K	Joback Method
tc	667.70	K	Joback Method
tf	290.51	K	Joback Method
vc	0.718	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	439.25	J/mol×K	508.48	Joback Method
cpg	451.54	J/mol×K	535.02	Joback Method
cpg	462.99	J/mol×K	561.55	Joback Method
cpg	473.63	J/mol×K	588.09	Joback Method
cpg	483.51	J/mol×K	614.63	Joback Method
cpg	492.67	J/mol×K	641.17	Joback Method
cpg	501.16	J/mol×K	667.70	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=R183745&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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