

Perfluoro-pentan ethioic acid S-propyl ester

Inchi:	InChI=1S/C8H7F9OS/c1-2-3-19-4(18)5(9,10)6(11,12)7(13,14)8(15,16)17/h2-3H2,1H3
InchiKey:	FVAPAUPI SNCB RP-UHFFFAOYSA-N
Formula:	C8H7F9OS
SMILES:	CCCSC(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]:	322.19

Physical Properties

Property code	Value	Unit	Source
gf	-1821.25	kJ/mol	Joback Method
hf	-2079.15	kJ/mol	Joback Method
hfus	20.27	kJ/mol	Joback Method
hvap	34.43	kJ/mol	Joback Method
log10ws	-4.43		Crippen Method
logp	4.124		Crippen Method
mcvol	157.430	ml/mol	McGowan Method
pc	2001.91	kPa	Joback Method
rinpol	851.00		NIST Webbook
rinpol	838.00		NIST Webbook
rinpol	854.00		NIST Webbook
rinpol	847.00		NIST Webbook
rinpol	854.00		NIST Webbook
ripol	869.00		NIST Webbook
ripol	952.00		NIST Webbook
ripol	923.00		NIST Webbook
ripol	897.00		NIST Webbook
tb	485.60	K	Joback Method
tc	645.50	K	Joback Method
tf	279.24	K	Joback Method
vc	0.661	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	394.17	J/mol×K	485.60	Joback Method

cpg	405.97	J/mol×K	512.25	Joback Method
cpg	416.92	J/mol×K	538.90	Joback Method
cpg	427.07	J/mol×K	565.55	Joback Method
cpg	436.46	J/mol×K	592.20	Joback Method
cpg	445.14	J/mol×K	618.85	Joback Method
cpg	453.15	J/mol×K	645.50	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=R183790&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
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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