Perfluoro-pentan ethioic acid S-pentyl ester

Inchi: InChI=1S/C10H11F9OS/c1-2-3-4-5-21-6(20)7(11,12)8(13,14)9(15,16)10(17,18)19/h2-5H
InchiKey: NJYRWUMITCPWHB-UHFFFAOYSA-N
Formula: C10H11F9OS
SMILES: CCCCCSC(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 350.24

Physical Properties

Property code	Value	Unit	Source
gf	-1804.41	kJ/mol	Joback Method
hf	-2120.43	kJ/mol	Joback Method
hfus	25.45	kJ/mol	Joback Method
hvap	38.88	kJ/mol	Joback Method
log10ws	-5.27		Crippen Method
logp	4.905		Crippen Method
mcvol	185.610	ml/mol	McGowan Method
pc	1697.70	kPa	Joback Method
rinpol	1026.00		NIST Webbook
rinpol	1034.00		NIST Webbook
rinpol	1041.00		NIST Webbook
rinpol	1041.00		NIST Webbook
ripol	1050.00		NIST Webbook
ripol	1109.00		NIST Webbook
ripol	1109.00		NIST Webbook
ripol	1080.00		NIST Webbook
ripol	1055.00		NIST Webbook
tb	531.36	K	Joback Method
tc	690.02	K	Joback Method
tf	301.78	K	Joback Method
vc	0.773	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	485.90	J/mol×K	531.36	Joback Method

cpg	498.64	J/mol×K	557.80	Joback Method
cpg	510.54	J/mol×K	584.25	Joback Method
cpg	521.62	J/mol×K	610.69	Joback Method
cpg	531.94	J/mol×K	637.13	Joback Method
cpg	541.54	J/mol×K	663.58	Joback Method
cpg	550.46	J/mol×K	690.02	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=R183785&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