perfluoro-pentan ethioic acid S-methyl ester

Inchi: InChI=1S/C6H3F9OS/c1-17-2(16)3(7,8)4(9,10)5(11,12)6(13,14)15/h1H3
InchiKey: MPMHHWHCHAJXRK-UHFFFAOYSA-N
Formula: C6H3F9OS
SMILES: CSC(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 294.14

Physical Properties

Property code	Value	Unit	Source
gf	-1838.09	kJ/mol	Joback Method
hf	-2037.87	kJ/mol	Joback Method
hfus	15.09	kJ/mol	Joback Method
hvap	29.98	kJ/mol	Joback Method
log10ws	-3.60		Crippen Method
logp	3.344		Crippen Method
mcvol	129.250	ml/mol	McGowan Method
pc	2395.87	kPa	Joback Method
tb	439.84	K	Joback Method
tc	601.15	K	Joback Method
tf	256.70	K	Joback Method
vc	0.549	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	309.08	J/mol×K	439.84	Joback Method
cpg	319.70	J/mol×K	466.73	Joback Method
cpg	329.49	J/mol×K	493.61	Joback Method
cpg	338.49	J/mol×K	520.50	Joback Method
cpg	346.75	J/mol×K	547.38	Joback Method
cpg	354.31	J/mol×K	574.27	Joback Method
cpg	361.21	J/mol×K	601.15	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R183770&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume