Perfluoro-pentan ethioic acid S-ethyl ester

Inchi: InChI=1S/C7H5F9OS/c1-2-18-3(17)4(8,9)5(10,11)6(12,13)7(14,15)16/h2H2,1H3
InchiKey: VIZPJQZIXDOYQY-UHFFFAOYSA-N
Formula: C7H5F9OS
SMILES: CCSC(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 308.17

Physical Properties

Property code	Value	Unit	Source
gf	-1829.67	kJ/mol	Joback Method
hf	-2058.51	kJ/mol	Joback Method
hfus	17.68	kJ/mol	Joback Method
hvap	32.20	kJ/mol	Joback Method
log10ws	-4.02		Crippen Method
logp	3.734		Crippen Method
mcvol	143.340	ml/mol	McGowan Method
pc	2185.64	kPa	Joback Method
rinpol	773.00		NIST Webbook
rinpol	766.00		NIST Webbook
rinpol	752.00		NIST Webbook
rinpol	757.00		NIST Webbook
ripol	880.00		NIST Webbook
ripol	821.00		NIST Webbook
ripol	855.00		NIST Webbook
ripol	797.00		NIST Webbook
tb	462.72	K	Joback Method
tc	623.33	K	Joback Method
tf	267.97	K	Joback Method
vc	0.606	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	350.75	J/mol×K	462.72	Joback Method
cpg	361.99	J/mol×K	489.49	Joback Method

cpg	372.39	J/mol×K	516.26	Joback Method
cpg	382.00	J/mol×K	543.03	Joback Method
cpg	390.86	J/mol×K	569.80	Joback Method
cpg	399.00	J/mol×K	596.56	Joback Method
cpg	406.49	J/mol×K	623.33	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R183750&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

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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