Perfluoro-pentan ethioic acid S-hexyl ester

Inchi: InChI=1S/C11H13F9OS/c1-2-3-4-5-6-22-7(21)8(12,13)9(14,15)10(16,17)11(18,19)20/h2-
InchiKey: PRQRSELZKXTBTC-UHFFFAOYSA-N
Formula: C11H13F9OS
SMILES: CCCCCCSC(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 364.27

Physical Properties

Property code	Value	Unit	Source
gf	-1795.99	kJ/mol	Joback Method
hf	-2141.07	kJ/mol	Joback Method
hfus	28.04	kJ/mol	Joback Method
hvap	41.11	kJ/mol	Joback Method
log10ws	-5.69		Crippen Method
logp	5.295		Crippen Method
mcvol	199.700	ml/mol	McGowan Method
pc	1570.96	kPa	Joback Method
rinpol	1138.00		NIST Webbook
rinpol	1138.00		NIST Webbook
rinpol	1131.00		NIST Webbook
rinpol	1124.00		NIST Webbook
ripol	1150.00		NIST Webbook
ripol	1207.00		NIST Webbook
ripol	1154.00		NIST Webbook
ripol	1180.00		NIST Webbook
ripol	1207.00		NIST Webbook
tb	554.24	K	Joback Method
tc	712.50	K	Joback Method
tf	313.05	K	Joback Method
vc	0.830	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	534.04	J/mol×K	554.24	Joback Method

cpg	547.19	J/mol×K	580.62	Joback Method
cpg	559.49	J/mol×K	606.99	Joback Method
cpg	570.97	J/mol×K	633.37	Joback Method
cpg	581.69	J/mol×K	659.75	Joback Method
cpg	591.69	J/mol×K	686.12	Joback Method
cpg	601.02	J/mol×K	712.50	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R183765&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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