Pentafluoropropanamide, N-heptyl-

Inchi: InChI=1S/C10H16F5NO/c1-2-3-4-5-6-7-16-8(17)9(11,12)10(13,14)15/h2-7H2,1H3,(H,16,
InchiKey: MYLVTEVOHVIWRU-UHFFFAOYSA-N
Formula: C10H16F5NO
SMILES: CCCCCCCNC(=O)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 261.23

Physical Properties

Property code	Value	Unit	Source
gf	-974.58	kJ/mol	Joback Method
hf	-1306.89	kJ/mol	Joback Method
hfus	28.93	kJ/mol	Joback Method
hvap	44.36	kJ/mol	Joback Method
log10ws	-3.95		Crippen Method
logp	3.271		Crippen Method
mcvol	172.160	ml/mol	McGowan Method
pc	1908.57	kPa	Joback Method
rinpol	1185.00		NIST Webbook
rinpol	1185.00		NIST Webbook
tb	522.13	K	Joback Method
tc	678.95	K	Joback Method
tf	312.84	K	Joback Method
vc	0.705	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	440.83	J/mol×K	522.13	Joback Method
cpg	454.15	J/mol×K	548.27	Joback Method
cpg	466.77	J/mol×K	574.40	Joback Method
cpg	478.73	J/mol×K	600.54	Joback Method
cpg	490.04	J/mol×K	626.68	Joback Method
cpg	500.74	J/mol×K	652.82	Joback Method
cpg	510.86	J/mol×K	678.95	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=U407337&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume