Pentafluoropropanamide, N-octyl-

Inchi: InChI=1S/C11H18F5NO/c1-2-3-4-5-6-7-8-17-9(18)10(12,13)11(14,15)16/h2-8H2,1H3,(H,
InchiKey: IVJJCCWXLNBFMZ-UHFFFAOYSA-N
Formula: C11H18F5NO
SMILES: CCCCCCCCNC(=O)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 275.26

Physical Properties

Property code	Value	Unit	Source
gf	-966.16	kJ/mol	Joback Method
hf	-1327.53	kJ/mol	Joback Method
hfus	31.52	kJ/mol	Joback Method
hvap	46.58	kJ/mol	Joback Method
log10ws	-4.37		Crippen Method
logp	3.661		Crippen Method
mcvol	186.250	ml/mol	McGowan Method
pc	1758.02	kPa	Joback Method
rinpol	1280.00		NIST Webbook
rinpol	1280.00		NIST Webbook
tb	545.01	K	Joback Method
tc	701.50	K	Joback Method
tf	324.11	K	Joback Method
vc	0.760	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	489.16	J/mol×K	545.01	Joback Method
cpg	503.03	J/mol×K	571.09	Joback Method
cpg	516.18	J/mol×K	597.17	Joback Method
cpg	528.64	J/mol×K	623.25	Joback Method
cpg	540.44	J/mol×K	649.33	Joback Method
cpg	551.62	J/mol×K	675.41	Joback Method
cpg	562.21	J/mol×K	701.50	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U407338&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume