Pentafluoropropanamide, N-octadecyl-

Inchi: InChI=1S/C21H38F5NO/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-27-19(28)20(22
InchiKey: HQPKNNKGXWPYGF-UHFFFAOYSA-N
Formula: C21H38F5NO
SMILES: CCCCCCCCCCCCCCCCCCNC(=O)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 415.52

Physical Properties

Property code	Value	Unit	Source
gf	-881.96	kJ/mol	Joback Method
hf	-1533.93	kJ/mol	Joback Method
hfus	57.42	kJ/mol	Joback Method
hvap	68.84	kJ/mol	Joback Method
log10ws	-8.55		Crippen Method
logp	7.562		Crippen Method
mcvol	327.150	ml/mol	McGowan Method
pc	893.73	kPa	Joback Method
rinpol	2229.00		NIST Webbook
rinpol	2229.00		NIST Webbook
tb	773.81	K	Joback Method
tc	947.49	K	Joback Method
tf	436.81	K	Joback Method
vc	1.321	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1044.14	J/mol×K	773.81	Joback Method
cpg	1062.79	J/mol×K	802.76	Joback Method
cpg	1080.45	J/mol×K	831.70	Joback Method
cpg	1097.20	J/mol×K	860.65	Joback Method
cpg	1113.10	J/mol×K	889.60	Joback Method
cpg	1128.20	J/mol×K	918.55	Joback Method
cpg	1142.56	J/mol×K	947.49	Joback Method

Sources

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=U407343&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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