Pentafluoropropanamide, N,N-dinonyl-

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

Physical Properties

Property code	Value	Unit	Source
gf	-860.57	kJ/mol	Joback Method
hf	-1519.87	kJ/mol	Joback Method
hfus	55.34	kJ/mol	Joback Method
hvap	64.45	kJ/mol	Joback Method
log10ws	-7.93		Crippen Method
logp	7.514		Crippen Method
mcvol	327.150	ml/mol	McGowan Method
pc	885.77	kPa	Joback Method
rinpol	2084.00		NIST Webbook
rinpol	2084.00		NIST Webbook
tb	736.08	K	Joback Method
tc	902.04	K	Joback Method
tf	416.62	K	Joback Method
vc	1.304	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1019.98	J/mol×K	736.08	Joback Method
cpg	1039.04	J/mol×K	763.74	Joback Method
cpg	1057.12	J/mol×K	791.40	Joback Method
cpg	1074.30	J/mol×K	819.06	Joback Method
cpg	1090.62	J/mol×K	846.72	Joback Method
cpg	1106.14	J/mol×K	874.38	Joback Method
cpg	1120.92	J/mol×K	902.04	Joback Method

Sources

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=U308516&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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