

Pentafluoropropanamide, N-nonyl-

Inchi:	InChI=1S/C12H20F5NO/c1-2-3-4-5-6-7-8-9-18-10(19)11(13,14)12(15,16)17/h2-9H2,1H3
InchiKey:	NWUCHZIGQDOFJA-UHFFFAOYSA-N
Formula:	C12H20F5NO
SMILES:	CCCCCCCCCNC(=O)C(F)(F)C(F)(F)F
Mol. weight [g/mol]:	289.29

Physical Properties

Property code	Value	Unit	Source
gf	-957.74	kJ/mol	Joback Method
hf	-1348.17	kJ/mol	Joback Method
hfus	34.11	kJ/mol	Joback Method
hvap	48.81	kJ/mol	Joback Method
log10ws	-4.79		Crippen Method
logp	4.051		Crippen Method
mcvol	200.340	ml/mol	McGowan Method
pc	1624.60	kPa	Joback Method
rinpol	1372.00		NIST Webbook
rinpol	1372.00		NIST Webbook
tb	567.89	K	Joback Method
tc	724.24	K	Joback Method
tf	335.38	K	Joback Method
vc	0.817	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	539.04	J/mol×K	567.89	Joback Method
cpg	553.41	J/mol×K	593.95	Joback Method
cpg	567.04	J/mol×K	620.01	Joback Method
cpg	579.97	J/mol×K	646.07	Joback Method
cpg	592.23	J/mol×K	672.12	Joback Method
cpg	603.85	J/mol×K	698.18	Joback Method
cpg	614.86	J/mol×K	724.24	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U407339&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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
h vap:	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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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