Pentafluoropropionic acid, nonyl ester

Other names: Nonyl pentafluoropropionate
Inchi: InChI=1S/C12H19F5O2/c1-2-3-4-5-6-7-8-9-19-10(18)11(13,14)12(15,16)17/h2-9H2,1H3
InchiKey: ZZUHMTSDSRPSDK-UHFFFAOYSA-N
Formula: C12H19F5O2
SMILES: CCCCCCCCCOC(=O)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 290.27
CAS: 959100-35-7

Physical Properties

Property code	Value	Unit	Source
gf	-1152.13	kJ/mol	Joback Method
hf	-1533.86	kJ/mol	Joback Method
hfus	30.19	kJ/mol	Joback Method
hvap	44.78	kJ/mol	Joback Method
log10ws	-4.68		Crippen Method
logp	4.478		Crippen Method
mcvol	196.230	ml/mol	McGowan Method
pc	1586.01	kPa	Joback Method
rinpol	1160.00		NIST Webbook
rinpol	1173.70		NIST Webbook
rinpol	1168.00		NIST Webbook
ripol	1215.00		NIST Webbook
tb	540.14	K	Joback Method
tc	693.05	K	Joback Method
tf	304.95	K	Joback Method
vc	0.799	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	510.59	J/mol×K	540.14	Joback Method
cpg	524.87	J/mol×K	565.63	Joback Method
cpg	538.47	J/mol×K	591.11	Joback Method
cpg	551.42	J/mol×K	616.60	Joback Method

cpg	563.75	J/mol×K	642.08	Joback Method
cpg	575.48	J/mol×K	667.57	Joback Method
cpg	586.63	J/mol×K	693.05	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C959100357&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume