Nonyl trifluoroacetate

Other names:	Nonyl trifluoroacetate
	Trifluoroacetic acid, nonyl ester
Inchi:	InChI=1S/C11H19F3O2/c1-2-3-4-5-6-7-8-9-16-10(15)11(12,13)14/h2-9H2,1H3
InchiKey:	ISEFXJGKOUSKCC-UHFFFAOYSA-N
Formula:	C11H19F3O2
SMILES:	CCCCCCCCCOC(=O)C(F)(F)F
Mol. weight [g/mol]:	240.27

Physical Properties

Property code	Value	Unit	Source
af	0.6254		Cheméo Relay (1.0)
hf	-1164.60	kJ/mol	Cheméo Relay (1.0)
hfus	28.86	kJ/mol	Joback Method
hvap	59.34	kJ/mol	Cheméo Relay (1.0)
ie	10.53	eV	Cheméo Relay (1.0)
log10ws	-3.91		Cheméo Relay (1.0)
logp	3.842		Crippen Method
mcvol	178.600	ml/mol	McGowan Method
pc	1820.06	kPa	Joback Method
rinpol	1156.70		NIST Webbook
rinpol	1153.00		NIST Webbook
rinpol	1156.70		NIST Webbook
rinpol	1176.30		NIST Webbook
rinpol	1153.00		NIST Webbook
rinpol	1137.00		NIST Webbook
rinpol	1123.60		NIST Webbook
ripol	1270.00		NIST Webbook
ripol	1270.00		NIST Webbook
tb	463.05	K	Cheméo Relay (1.0)
tc	586.09	K	Cheméo Relay (1.0)
tf	237.78	K	Cheméo Relay (1.0)
vc	0.683	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	442.66	J/mol×K	521.95	Joback Method
cpg	456.65	J/mol×K	548.33	Joback Method
cpg	470.04	J/mol×K	574.70	Joback Method
cpg	482.85	J/mol×K	601.08	Joback Method
cpg	495.10	J/mol×K	627.45	Joback Method
cpg	506.80	J/mol×K	653.83	Joback Method
cpg	517.97	J/mol×K	680.20	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C30767147&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method

Legend

af: Acentric Factor
cpg: Ideal gas heat capacity
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hvap: Enthalpy of vaporization at standard conditions
ie: Ionization energy
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