

Acetic acid, trifluoro-, nonyl ester

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]:	240.26
CAS:	30767-14-7

Physical Properties

Property code	Value	Unit	Source
gf	-773.77	kJ/mol	Joback Method
hf	-1112.25	kJ/mol	Joback Method
hfus	28.86	kJ/mol	Joback Method
hvap	45.49	kJ/mol	Joback Method
log10ws	-3.95		Crippen Method
logp	3.842		Crippen Method
mcvol	178.600	ml/mol	McGowan Method
pc	1820.06	kPa	Joback Method
rinpol	1123.60		NIST Webbook
rinpol	1153.00		NIST Webbook
rinpol	1176.30		NIST Webbook
rinpol	1156.70		NIST Webbook
rinpol	1153.00		NIST Webbook
rinpol	1137.00		NIST Webbook
rinpol	1156.70		NIST Webbook
ripol	1270.00		NIST Webbook
ripol	1270.00		NIST Webbook
tb	521.95	K	Joback Method
tc	680.20	K	Joback Method
tf	290.08	K	Joback Method
vc	0.719	m ³ /kmol	Joback Method

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C30767147&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.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
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

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