Nonanoic acid, 2,2,2-trichloroethyl ester

Other names: 2,2,2-Trichloroethyl nonanoate
Inchi: InChI=1S/C11H19Cl3O2/c1-2-3-4-5-6-7-8-10(15)16-9-11(12,13)14/h2-9H2,1H3
InchiKey: UNSPRHCUPSMXLE-UHFFFAOYSA-N
Formula: C11H19Cl3O2
SMILES: CCCCCCCCC(=O)OCC(Cl)(Cl)Cl
Mol. weight [g/mol]: 289.63

Physical Properties

Property code	Value	Unit	Source
gf	-225.13	kJ/mol	Joback Method
hf	-571.14	kJ/mol	Joback Method
hfus	32.21	kJ/mol	Joback Method
hvap	61.09	kJ/mol	Joback Method
log10ws	-4.85		Crippen Method
logp	4.650		Crippen Method
mcvol	210.010	ml/mol	McGowan Method
pc	1857.91	kPa	Joback Method
rinpol	1694.00		NIST Webbook
rinpol	1660.00		NIST Webbook
rinpol	1675.00		NIST Webbook
rinpol	1674.00		NIST Webbook
rinpol	1678.00		NIST Webbook
rinpol	1660.00		NIST Webbook
rinpol	1676.00		NIST Webbook
rinpol	1679.00		NIST Webbook
rinpol	1679.00		NIST Webbook
rinpol	1678.00		NIST Webbook
rinpol	1694.00		NIST Webbook
ripol	2058.00		NIST Webbook
ripol	2045.00		NIST Webbook
ripol	2040.00		NIST Webbook
ripol	2090.00		NIST Webbook
ripol	2026.00		NIST Webbook
ripol	2039.00		NIST Webbook
ripol	2039.00		NIST Webbook
ripol	2026.00		NIST Webbook
ripol	2090.00		NIST Webbook

ripol	2065.00		NIST Webbook
tb	636.43	K	Joback Method
tc	830.26	K	Joback Method
tf	378.07	K	Joback Method
vc	0.811	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	507.77	J/mol×K	636.43	Joback Method
cpg	567.74	J/mol×K	797.96	Joback Method
cpg	557.15	J/mol×K	765.65	Joback Method
cpg	545.89	J/mol×K	733.35	Joback Method
cpg	533.93	J/mol×K	701.04	Joback Method
cpg	521.23	J/mol×K	668.74	Joback Method
cpg	577.68	J/mol×K	830.26	Joback Method
dvisc	0.0001454	Pa×s	636.43	Joback Method
dvisc	0.0001927	Pa×s	593.37	Joback Method
dvisc	0.0002668	Pa×s	550.31	Joback Method
dvisc	0.0003905	Pa×s	507.25	Joback Method
dvisc	0.0006134	Pa×s	464.19	Joback Method
dvisc	0.0010567	Pa×s	421.13	Joback Method
dvisc	0.0020603	Pa×s	378.07	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U360667&Units=SI

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity

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