

Trichloroacetic acid, undec-2-enyl ester

Inchi:	InChI=1S/C13H21Cl3O2/c1-2-3-4-5-6-7-8-9-10-11-18-12(17)13(14,15)16/h9-10H,2-8,11H
InchiKey:	HPCFGWRDJUTDBB-MDZDMXLPSA-N
Formula:	C13H21Cl3O2
SMILES:	CCCCCCCCC=CCOC(=O)C(Cl)(Cl)Cl
Mol. weight [g/mol]:	315.66

Physical Properties

Property code	Value	Unit	Source
gf	-128.07	kJ/mol	Joback Method
hf	-495.20	kJ/mol	Joback Method
hfus	37.59	kJ/mol	Joback Method
hvap	65.50	kJ/mol	Joback Method
log10ws	-5.54		Crippen Method
logp	5.207		Crippen Method
mvol	233.890	ml/mol	McGowan Method
pc	1652.46	kPa	Joback Method
rinpol	1859.00		NIST Webbook
tb	686.35	K	Joback Method
tc	882.83	K	Joback Method
tf	395.53	K	Joback Method
vc	0.903	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	588.67	J/molxK	686.35	Joback Method
cpg	602.60	J/molxK	719.10	Joback Method
cpg	615.70	J/molxK	751.84	Joback Method
cpg	628.03	J/molxK	784.59	Joback Method
cpg	639.63	J/molxK	817.34	Joback Method
cpg	650.55	J/molxK	850.08	Joback Method
cpg	660.85	J/molxK	882.83	Joback Method
dvisc	0.0015726	Paxs	395.53	Joback Method
dvisc	0.0007602	Paxs	444.00	Joback Method

dvisc	0.0004240	Paxs	492.47	Joback Method
dvisc	0.0002626	Paxs	540.94	Joback Method
dvisc	0.0001760	Paxs	589.41	Joback Method
dvisc	0.0001253	Paxs	637.88	Joback Method
dvisc	0.0000936	Paxs	686.35	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299261&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

cp_g:	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:	Log ₁₀ of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
m_{cvol}:	McGowan's characteristic volume
pc:	Critical Pressure
rin_{pol}:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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