

Trichloroacetic acid, tridecyl ester

Other names:	Tridecyl trichloroacetate
Inchi:	InChI=1S/C15H27Cl3O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-20-14(19)15(16,17)18/h2-13H2
InchiKey:	IVESCNMAOKRZNG-UHFFFAOYSA-N
Formula:	C15H27Cl3O2
SMILES:	CCCCCCCCCCCCCOC(=O)C(Cl)(Cl)Cl
Mol. weight [g/mol]:	345.73
CAS:	74339-51-8

Physical Properties

Property code	Value	Unit	Source
gf	-191.45	kJ/mol	Joback Method
hf	-653.70	kJ/mol	Joback Method
hfus	42.57	kJ/mol	Joback Method
hvap	70.00	kJ/mol	Joback Method
log10ws	-6.53		Crippen Method
logp	6.211		Crippen Method
mcvol	266.370	ml/mol	McGowan Method
pc	1367.69	kPa	Joback Method
rinpol	2071.00		NIST Webbook
tb	727.95	K	Joback Method
tc	915.98	K	Joback Method
tf	423.15	K	Joback Method
vc	1.036	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	719.98	J/molxK	727.95	Joback Method
cpg	735.27	J/molxK	759.29	Joback Method
cpg	749.70	J/molxK	790.63	Joback Method
cpg	763.32	J/molxK	821.96	Joback Method
cpg	776.15	J/molxK	853.30	Joback Method
cpg	788.25	J/molxK	884.64	Joback Method
cpg	799.64	J/molxK	915.98	Joback Method

dvisc	0.0013475	Paxs	423.15	Joback Method
dvisc	0.0006554	Paxs	473.95	Joback Method
dvisc	0.0003665	Paxs	524.75	Joback Method
dvisc	0.0002271	Paxs	575.55	Joback Method
dvisc	0.0001521	Paxs	626.35	Joback Method
dvisc	0.0001082	Paxs	677.15	Joback Method
dvisc	0.0000807	Paxs	727.95	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C74339518&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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
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
mvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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