

Trichloroacetic acid, triethylene glycol diester

Inchi: InChI=1S/C10H12Cl6O6/c11-9(12,13)7(17)21-5-3-19-1-2-20-4-6-22-8(18)10(14,15)16/h1
InchiKey: RIJPRJBXZMWTK-UHFFFAOYSA-N
Formula: C10H12Cl6O6
SMILES: O=C(OCCOCCOCCOC(=O)C(Cl)(Cl)Cl)C(Cl)(Cl)Cl
Mol. weight [g/mol]: 440.92

Physical Properties

Property code	Value	Unit	Source
gf	-710.42	kJ/mol	Joback Method
hf	-1115.71	kJ/mol	Joback Method
hfus	39.96	kJ/mol	Joback Method
hvap	84.70	kJ/mol	Joback Method
log10ws	-3.03		Crippen Method
logp	2.846		Crippen Method
mcvol	251.820	ml/mol	McGowan Method
pc	1883.80	kPa	Joback Method
tb	843.74	K	Joback Method
tc	1062.03	K	Joback Method
tf	575.60	K	Joback Method
vc	0.952	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	611.51	J/molxK	843.74	Joback Method
cpg	619.49	J/molxK	880.12	Joback Method
cpg	626.62	J/molxK	916.50	Joback Method
cpg	632.91	J/molxK	952.89	Joback Method
cpg	638.38	J/molxK	989.27	Joback Method
cpg	643.05	J/molxK	1025.65	Joback Method
cpg	646.93	J/molxK	1062.03	Joback Method
dvisc	0.0002435	Paxs	575.60	Joback Method
dvisc	0.0001524	Paxs	620.29	Joback Method
dvisc	0.0001016	Paxs	664.98	Joback Method

dvisc	0.0000713	Paxs	709.67	Joback Method
dvisc	0.0000522	Paxs	754.36	Joback Method
dvisc	0.0000395	Paxs	799.05	Joback Method
dvisc	0.0000308	Paxs	843.74	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=B6002374&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
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvac:	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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:

<https://www.chemeo.com/cid/94-277-1/Trichloroacetic-acid-triethylene-glycol-diester.pdf>

Generated by Cheméo on 2024-04-26 17:01:31.939316417 +0000 UTC m=+16440140.859893766.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.