Trichloroacetic acid, dodecyl ester

Other names: Dodecyl trichloroacetate
Inchi: InChI=1S/C14H25Cl3O2/c1-2-3-4-5-6-7-8-9-10-11-12-19-13(18)14(15,16)17/h2-12H2,1H
InchiKey: LFBVFMYQESVNJY-UHFFFAOYSA-N
Formula: C14H25Cl3O2
SMILES: CCCCCCCCCCCCOC(=O)C(Cl)(Cl)Cl
Mol. weight [g/mol]: 331.71
CAS: 74339-50-7

Physical Properties

Property code	Value	Unit	Source
gf	-199.87	kJ/mol	Joback Method
hf	-633.06	kJ/mol	Joback Method
hfus	39.98	kJ/mol	Joback Method
hvap	67.77	kJ/mol	Joback Method
log10ws	-6.11		Crippen Method
logp	5.821		Crippen Method
mcvol	252.280	ml/mol	McGowan Method
pc	1470.23	kPa	Joback Method
rinpol	1963.00		NIST Webbook
rinpol	1966.00		NIST Webbook
rinpol	1963.00		NIST Webbook
rinpol	1966.00		NIST Webbook
rinpol	1971.00		NIST Webbook
ripol	2369.00		NIST Webbook
ripol	2369.00		NIST Webbook
tb	705.07	K	Joback Method
tc	893.91	K	Joback Method
tf	411.88	K	Joback Method
vc	0.980	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	665.06	J/mol×K	705.07	Joback Method

cpg	679.96	J/mol×K	736.54	Joback Method
cpg	694.02	J/mol×K	768.02	Joback Method
cpg	707.28	J/mol×K	799.49	Joback Method
cpg	719.78	J/mol×K	830.96	Joback Method
cpg	731.56	J/mol×K	862.44	Joback Method
cpg	742.64	J/mol×K	893.91	Joback Method
dvisc	0.0015087	Pa×s	411.88	Joback Method
dvisc	0.0007429	Pa×s	460.75	Joback Method
dvisc	0.0004190	Pa×s	509.61	Joback Method
dvisc	0.0002613	Pa×s	558.47	Joback Method
dvisc	0.0001758	Pa×s	607.34	Joback Method
dvisc	0.0001254	Pa×s	656.20	Joback Method
dvisc	0.0000938	Pa×s	705.07	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C74339507&Units=SI
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

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