2,2,2-Trichloroethyl tridecanoate

Inchi: InChI=1S/C15H27Cl3O2/c1-2-3-4-5-6-7-8-9-10-11-12-14(19)20-13-15(16,17)18/h2-13H2
InchiKey: VXYPICBEGVDWKX-UHFFFAOYSA-N
Formula: C15H27Cl3O2
SMILES: CCCCCCCCCCCCC(=O)OCC(Cl)(Cl)Cl
Mol. weight [g/mol]: 345.73

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	2077.00		NIST Webbook
rinpol	2076.00		NIST Webbook
rinpol	2074.00		NIST Webbook
rinpol	2074.00		NIST Webbook
ripol	2462.00		NIST Webbook
ripol	2467.00		NIST Webbook
ripol	2485.00		NIST Webbook
ripol	2452.00		NIST Webbook
ripol	2436.00		NIST Webbook
ripol	2440.00		NIST Webbook
ripol	2436.00		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/mol×K	727.95	Joback Method
cpg	735.27	J/mol×K	759.29	Joback Method
cpg	749.70	J/mol×K	790.63	Joback Method
cpg	763.32	J/mol×K	821.96	Joback Method
cpg	776.15	J/mol×K	853.30	Joback Method
cpg	788.25	J/mol×K	884.64	Joback Method
cpg	799.64	J/mol×K	915.98	Joback Method
dvisc	0.0013475	Pa×s	423.15	Joback Method
dvisc	0.0006554	Pa×s	473.95	Joback Method
dvisc	0.0003665	Pa×s	524.75	Joback Method
dvisc	0.0002271	Pa×s	575.55	Joback Method
dvisc	0.0001521	Pa×s	626.35	Joback Method
dvisc	0.0001082	Pa×s	677.15	Joback Method
dvisc	0.0000807	Pa×s	727.95	Joback Method

Sources

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=R30545&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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