2,2,2-Trichloroethyl heptanoate

Other names: Heptanoic acid, 2,2,2-trichloroethyl ester
Inchi: InChI=1S/C9H15Cl3O2/c1-2-3-4-5-6-8(13)14-7-9(10,11)12/h2-7H2,1H3
InchiKey: LBQWQJOXEYEDAX-UHFFFAOYSA-N
Formula: C9H15Cl3O2
SMILES: CCCCCCC(=O)OCC(Cl)(Cl)Cl
Mol. weight [g/mol]: 261.57

Physical Properties

Property code	Value	Unit	Source
gf	-241.97	kJ/mol	Joback Method
hf	-529.86	kJ/mol	Joback Method
hfus	27.03	kJ/mol	Joback Method
hvap	56.64	kJ/mol	Joback Method
log10ws	-4.01		Crippen Method
logp	3.870		Crippen Method
mcvol	181.830	ml/mol	McGowan Method
pc	2208.29	kPa	Joback Method
rinpol	1479.00		NIST Webbook
rinpol	1478.00		NIST Webbook
rinpol	1462.00		NIST Webbook
rinpol	1462.00		NIST Webbook
rinpol	1477.00		NIST Webbook
rinpol	1478.00		NIST Webbook
rinpol	1482.00		NIST Webbook
rinpol	1478.00		NIST Webbook
rinpol	1477.00		NIST Webbook
ripol	1850.00		NIST Webbook
ripol	1840.00		NIST Webbook
ripol	1832.00		NIST Webbook
ripol	1898.00		NIST Webbook
ripol	1854.00		NIST Webbook
ripol	1832.00		NIST Webbook
ripol	1898.00		NIST Webbook
ripol	1843.00		NIST Webbook
ripol	1874.00		NIST Webbook
tb	590.67	K	Joback Method
tc	789.49	K	Joback Method

tf	355.53	K	Joback Method
vc	0.700	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	409.97	J/mol×K	590.67	Joback Method
cpg	422.15	J/mol×K	623.81	Joback Method
cpg	433.62	J/mol×K	656.94	Joback Method
cpg	444.40	J/mol×K	690.08	Joback Method
cpg	454.53	J/mol×K	723.22	Joback Method
cpg	464.04	J/mol×K	756.36	Joback Method
cpg	472.95	J/mol×K	789.49	Joback Method
dvisc	0.0024677	Pa×s	355.53	Joback Method
dvisc	0.0013053	Pa×s	394.72	Joback Method
dvisc	0.0007746	Pa×s	433.91	Joback Method
dvisc	0.0005012	Pa×s	473.10	Joback Method
dvisc	0.0003466	Pa×s	512.29	Joback Method
dvisc	0.0002526	Pa×s	551.48	Joback Method
dvisc	0.0001920	Pa×s	590.67	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R19890&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