Trichloroacetic acid, hexyl ester

Other names: Hexyl trichloroacetate
Inchi: InChI=1S/C8H13Cl3O2/c1-2-3-4-5-6-13-7(12)8(9,10)11/h2-6H2,1H3
InchiKey: UJGLOWVVUOBEJU-UHFFFAOYSA-N
Formula: C8H13Cl3O2
SMILES: CCCCCCOC(=O)C(Cl)(Cl)Cl
Mol. weight [g/mol]: 247.55
CAS: 37587-86-3

Physical Properties

Property code	Value	Unit	Source
gf	-250.39	kJ/mol	Joback Method
hf	-509.22	kJ/mol	Joback Method
hfus	24.44	kJ/mol	Joback Method
hvap	54.42	kJ/mol	Joback Method
log10ws	-3.60		Crippen Method
logp	3.480		Crippen Method
mcvol	167.740	ml/mol	McGowan Method
pc	2421.88	kPa	Joback Method
rinpol	1350.00		NIST Webbook
rinpol	1358.00		NIST Webbook
rinpol	1361.00		NIST Webbook
rinpol	1367.00		NIST Webbook
rinpol	1315.00		NIST Webbook
rinpol	1359.00		NIST Webbook
rinpol	1380.00		NIST Webbook
rinpol	1339.70		NIST Webbook
rinpol	1366.70		NIST Webbook
rinpol	1372.00		NIST Webbook
rinpol	1353.00		NIST Webbook
rinpol	1353.00		NIST Webbook
rinpol	1315.00		NIST Webbook
rinpol	1340.00		NIST Webbook
rinpol	1372.00		NIST Webbook
rinpol	1340.00		NIST Webbook
ripol	1726.00		NIST Webbook
ripol	1734.00		NIST Webbook
ripol	1766.00		NIST Webbook

ripol	1741.00		NIST Webbook
ripol	1726.00		NIST Webbook
tb	567.79	K	Joback Method
tc	769.47	K	Joback Method
tf	344.26	K	Joback Method
vc	0.643	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	363.45	J/mol×K	567.79	Joback Method
cpg	374.85	J/mol×K	601.40	Joback Method
cpg	385.58	J/mol×K	635.02	Joback Method
cpg	395.65	J/mol×K	668.63	Joback Method
cpg	405.09	J/mol×K	702.24	Joback Method
cpg	413.95	J/mol×K	735.85	Joback Method
cpg	422.23	J/mol×K	769.47	Joback Method
dvisc	0.0026742	Pa×s	344.26	Joback Method
dvisc	0.0014383	Pa×s	381.51	Joback Method
dvisc	0.0008638	Pa×s	418.77	Joback Method
dvisc	0.0005639	Pa×s	456.02	Joback Method
dvisc	0.0003926	Pa×s	493.28	Joback Method
dvisc	0.0002876	Pa×s	530.53	Joback Method
dvisc	0.0002194	Pa×s	567.79	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C37587863&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

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