Cyclohexanecarboxylic acid, 2,2,2-trichloroethyl ester

Inchi: InChI=1S/C9H13Cl3O2/c10-9(11,12)6-14-8(13)7-4-2-1-3-5-7/h7H,1-6H2

InchiKey: LDNCHQISWJTDHK-UHFFFAOYSA-N

Formula: C9H13Cl3O2

SMILES: O=C(OCC(Cl)(Cl)Cl)C1CCCCC1

Mol. weight [g/mol]: 259.56

Physical Properties

Property code	Value	Unit	Source
gf	-217.52	kJ/mol	Joback Method
hf	-475.54	kJ/mol	Joback Method
hfus	18.86	kJ/mol	Joback Method
hvap	57.07	kJ/mol	Joback Method
log10ws	-3.67		Crippen Method
logp	3.480		Crippen Method
mcvol	170.970	ml/mol	McGowan Method
pc	2704.22	kPa	Joback Method
rinpol	1563.00		NIST Webbook
rinpol	1563.00		NIST Webbook
tb	610.22	K	Joback Method
tc	845.54	K	Joback Method
tf	362.91	K	Joback Method
vc	0.632	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	398.15	J/mol×K	610.22	Joback Method
cpg	462.45	J/mol×K	806.32	Joback Method
cpg	451.70	J/mol×K	767.10	Joback Method
cpg	439.95	J/mol×K	727.88	Joback Method
cpg	427.14	J/mol×K	688.66	Joback Method
cpg	413.22	J/mol×K	649.44	Joback Method
cpg	472.24	J/mol×K	845.54	Joback Method
dvisc	0.0002013	Pa×s	610.22	Joback Method

dvisc	0.0002678	Pa×s	569.00	Joback Method
dvisc	0.0003725	Pa×s	527.78	Joback Method
dvisc	0.0005479	Pa×s	486.57	Joback Method
dvisc	0.0008658	Pa×s	445.35	Joback Method
dvisc	0.0015018	Pa×s	404.13	Joback Method
dvisc	0.0029522	Pa×s	362.91	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U354650&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume