3-Cyclopentylpropionic acid, 2,2,2-trichloroethyl ester

Inchi: InChI=1S/C10H15Cl3O2/c11-10(12,13)7-15-9(14)6-5-8-3-1-2-4-8/h8H,1-7H2
InchiKey: FSBUEXBDAXOKOU-UHFFFAOYSA-N
Formula: C10H15Cl3O2
SMILES: O=C(CCC1CCCC1)OCC(Cl)(Cl)Cl
Mol. weight [g/mol]: 273.58

Physical Properties

Property code	Value	Unit	Source
gf	-197.00	kJ/mol	Joback Method
hf	-490.02	kJ/mol	Joback Method
hfus	23.55	kJ/mol	Joback Method
hvap	59.13	kJ/mol	Joback Method
log10ws	-4.09		Crippen Method
logp	3.870		Crippen Method
mcvol	185.060	ml/mol	McGowan Method
pc	2393.53	kPa	Joback Method
rinpol	1672.00		NIST Webbook
rinpol	1672.00		NIST Webbook
tb	628.83	K	Joback Method
tc	851.99	K	Joback Method
tf	377.70	K	Joback Method
vc	0.697	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	445.97	J/mol×K	628.83	Joback Method
cpg	460.76	J/mol×K	666.02	Joback Method
cpg	474.48	J/mol×K	703.22	Joback Method
cpg	487.18	J/mol×K	740.41	Joback Method
cpg	498.93	J/mol×K	777.60	Joback Method
cpg	509.78	J/mol×K	814.80	Joback Method
cpg	519.78	J/mol×K	851.99	Joback Method
dvisc	0.0026118	Pa×s	377.70	Joback Method

dvisc	0.0014281	Pa×s	419.56	Joback Method
dvisc	0.0008712	Pa×s	461.41	Joback Method
dvisc	0.0005770	Pa×s	503.27	Joback Method
dvisc	0.0004072	Pa×s	545.12	Joback Method
dvisc	0.0003019	Pa×s	586.98	Joback Method
dvisc	0.0002330	Pa×s	628.83	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=U354331&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume