2,2,2-Trichloroethyl «beta»-phenylpropionate

Other names: 3-Phenylpropionic acid, 2,2,2-trichloroethyl ester
Inchi: InChI=1S/C11H11Cl3O2/c12-11(13,14)8-16-10(15)7-6-9-4-2-1-3-5-9/h1-5H,6-8H2
InchiKey: ZUBQPTWQWDFBQU-UHFFFAOYSA-N
Formula: C11H11Cl3O2
SMILES: O=C(CCc1ccccc1)OCC(Cl)(Cl)Cl
Mol. weight [g/mol]: 281.56
CAS: 23522-65-8

Physical Properties

Property code	Value	Unit	Source
gf	-112.72	kJ/mol	Joback Method
hf	-334.61	kJ/mol	Joback Method
hfus	26.25	kJ/mol	Joback Method
hvap	63.37	kJ/mol	Joback Method
log10ws	-3.95		Crippen Method
logp	3.533		Crippen Method
mcvol	186.250	ml/mol	McGowan Method
pc	2527.73	kPa	Joback Method
rinpol	1800.00		NIST Webbook
tb	663.11	K	Joback Method
tc	896.34	K	Joback Method
tf	404.49	K	Joback Method
vc	0.704	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	426.42	J/mol×K	663.11	Joback Method
cpg	477.14	J/mol×K	857.47	Joback Method
cpg	468.73	J/mol×K	818.59	Joback Method
cpg	459.52	J/mol×K	779.72	Joback Method
cpg	449.44	J/mol×K	740.85	Joback Method
cpg	438.43	J/mol×K	701.98	Joback Method
cpg	484.81	J/mol×K	896.34	Joback Method

dvisc	0.0001428	Pa×s	663.11	Joback Method
dvisc	0.0001857	Pa×s	620.01	Joback Method
dvisc	0.0002510	Pa×s	576.90	Joback Method
dvisc	0.0003563	Pa×s	533.80	Joback Method
dvisc	0.0005378	Pa×s	490.70	Joback Method
dvisc	0.0008789	Pa×s	447.59	Joback Method
dvisc	0.0015947	Pa×s	404.49	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C23522658&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

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