Isovaleric acid, 2,3,4,6-tetrachlorophenyl ester

Inchi: InChI=1S/C11H10Cl4O2/c1-5(2)3-8(16)17-11-7(13)4-6(12)9(14)10(11)15/h4-5H,3H2,1-2
InchiKey: FGPHMRAXOBSQAS-UHFFFAOYSA-N
Formula: C11H10Cl4O2
SMILES: CC(C)CC(=O)Oc1c(Cl)cc(Cl)c(Cl)c1Cl
Mol. weight [g/mol]: 316.01

Physical Properties

Property code	Value	Unit	Source
gf	-168.45	kJ/mol	Joback Method
hf	-392.76	kJ/mol	Joback Method
hfus	32.78	kJ/mol	Joback Method
hvap	71.31	kJ/mol	Joback Method
log10ws	-5.54		Crippen Method
logp	5.252		Crippen Method
mcvol	198.490	ml/mol	McGowan Method
pc	2274.07	kPa	Joback Method
rinpol	1910.00		NIST Webbook
tb	723.25	K	Joback Method
tc	954.16	K	Joback Method
tf	467.07	K	Joback Method
vc	0.757	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	439.68	J/mol×K	723.25	Joback Method
cpg	449.98	J/mol×K	761.73	Joback Method
cpg	459.53	J/mol×K	800.22	Joback Method
cpg	468.34	J/mol×K	838.70	Joback Method
cpg	476.40	J/mol×K	877.19	Joback Method
cpg	483.74	J/mol×K	915.67	Joback Method
cpg	490.35	J/mol×K	954.16	Joback Method
dvisc	0.0007626	Pa×s	467.07	Joback Method
dvisc	0.0005079	Pa×s	509.77	Joback Method

dvisc	0.0003603	Pa×s	552.46	Joback Method
dvisc	0.0002684	Pa×s	595.16	Joback Method
dvisc	0.0002080	Pa×s	637.86	Joback Method
dvisc	0.0001665	Pa×s	680.55	Joback Method
dvisc	0.0001368	Pa×s	723.25	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U360659&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