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

Inchi: InChI=1S/C11H8Cl4O2/c12-6-4-7(13)10(9(15)8(6)14)17-11(16)5-2-1-3-5/h4-5H,1-3H2

InchiKey: QKTJMHLJOJEOJB-UHFFFAOYSA-N

Formula: C11H8Cl4O2

SMILES: O=C(Oc1c(Cl)cc(Cl)c(Cl)c1Cl)C1CCC1

Mol. weight [g/mol]: 313.99

Physical Properties

Property code	Value	Unit	Source
gf	-117.36	kJ/mol	Joback Method
hf	-320.84	kJ/mol	Joback Method
hfus	32.34	kJ/mol	Joback Method
hvap	71.78	kJ/mol	Joback Method
log10ws	-5.43		Crippen Method
logp	5.006		Crippen Method
mcvol	187.630	ml/mol	McGowan Method
pc	2629.85	kPa	Joback Method
rinpol	2064.00		NIST Webbook
rinpol	2064.00		NIST Webbook
tb	734.70	K	Joback Method
tc	983.25	K	Joback Method
tf	496.49	K	Joback Method
vc	0.713	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	424.22	J/mol×K	734.70	Joback Method
cpg	434.93	J/mol×K	776.13	Joback Method
cpg	444.74	J/mol×K	817.55	Joback Method
cpg	453.69	J/mol×K	858.98	Joback Method
cpg	461.83	J/mol×K	900.40	Joback Method
cpg	469.18	J/mol×K	941.83	Joback Method
cpg	475.79	J/mol×K	983.25	Joback Method
dvisc	0.0010583	Pa×s	496.49	Joback Method

dvisc	0.0007941	Pa×s	536.19	Joback Method
dvisc	0.0006200	Pa×s	575.89	Joback Method
dvisc	0.0004997	Pa×s	615.60	Joback Method
dvisc	0.0004134	Pa×s	655.30	Joback Method
dvisc	0.0003495	Pa×s	695.00	Joback Method
dvisc	0.0003009	Pa×s	734.70	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U355164&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