Cyclobutanecarboxylic acid, 2,4,5-trichlorophenyl ester

Inchi: InChI=1S/C11H9Cl3O2/c12-7-4-9(14)10(5-8(7)13)16-11(15)6-2-1-3-6/h4-6H,1-3H2

InchiKey: SRPUKOHZFYRNRV-UHFFFAOYSA-N

Formula: C11H9Cl3O2

SMILES: O=C(Oc1cc(Cl)c(Cl)cc1Cl)C1CCC1

Mol. weight [g/mol]: 279.55

Physical Properties

Property code	Value	Unit	Source
gf	-95.80	kJ/mol	Joback Method
hf	-293.63	kJ/mol	Joback Method
hfus	28.53	kJ/mol	Joback Method
hvap	66.74	kJ/mol	Joback Method
log10ws	-4.75		Crippen Method
logp	4.352		Crippen Method
mcvol	175.390	ml/mol	McGowan Method
pc	2775.92	kPa	Joback Method
rinpol	1923.00		NIST Webbook
rinpol	1923.00		NIST Webbook
tb	692.29	K	Joback Method
tc	937.83	K	Joback Method
tf	454.05	K	Joback Method
vc	0.663	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	404.51	J/mol×K	692.29	Joback Method
cpg	416.46	J/mol×K	733.21	Joback Method
cpg	427.47	J/mol×K	774.14	Joback Method
cpg	437.56	J/mol×K	815.06	Joback Method
cpg	446.79	J/mol×K	855.98	Joback Method
cpg	455.20	J/mol×K	896.91	Joback Method
cpg	462.83	J/mol×K	937.83	Joback Method
dvisc	0.0012695	Pa×s	454.05	Joback Method

dvisc	0.0009220	Pa×s	493.76	Joback Method
dvisc	0.0007023	Pa×s	533.46	Joback Method
dvisc	0.0005555	Pa×s	573.17	Joback Method
dvisc	0.0004530	Pa×s	612.88	Joback Method
dvisc	0.0003786	Pa×s	652.58	Joback Method
dvisc	0.0003231	Pa×s	692.29	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U355163&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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