

4-Tert-butylphenyl 2,2-dichloropropanoate

Inchi:	InChI=1S/C13H16Cl2O2/c1-12(2,3)9-5-7-10(8-6-9)17-11(16)13(4,14)15/h5-8H,1-4H3
InchiKey:	MJPDDYAFICYSHHG-UHFFFAOYSA-N
Formula:	C13H16Cl2O2
SMILES:	CC(Cl)(Cl)C(=O)Oc1ccc(C(C)(C)C)cc1
Mol. weight [g/mol]:	275.17
CAS:	116594-65-1

Physical Properties

Property code	Value	Unit	Source
gf	-90.74	kJ/mol	Joback Method
hf	-380.37	kJ/mol	Joback Method
hfus	19.43	kJ/mol	Joback Method
hvap	62.80	kJ/mol	Joback Method
log10ws	-4.43		Crippen Method
logp	4.083		Crippen Method
mcvol	202.190	ml/mol	McGowan Method
pc	2183.60	kPa	Joback Method
tb	673.19	K	Joback Method
tc	908.60	K	Joback Method
tf	412.05	K	Joback Method
vc	0.755	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	504.08	J/molxK	673.19	Joback Method
cpg	518.72	J/molxK	712.43	Joback Method
cpg	532.16	J/molxK	751.66	Joback Method
cpg	544.51	J/molxK	790.90	Joback Method
cpg	555.85	J/molxK	830.13	Joback Method
cpg	566.27	J/molxK	869.37	Joback Method
cpg	575.86	J/molxK	908.60	Joback Method
dvisc	0.0013322	Paxs	412.05	Joback Method
dvisc	0.0007109	Paxs	455.57	Joback Method

dvisc	0.0004233	Paxs	499.10	Joback Method
dvisc	0.0002739	Paxs	542.62	Joback Method
dvisc	0.0001891	Paxs	586.14	Joback Method
dvisc	0.0001374	Paxs	629.67	Joback Method
dvisc	0.0001040	Paxs	673.19	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=C116594651&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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