

(5-Tert-butyl-2-hydroxyphenyl)(3,4-dichlorophenyl)propanoate

Inchi:	InChI=1S/C17H16Cl2O2/c1-17(2,3)11-5-7-15(20)12(9-11)16(21)10-4-6-13(18)14(19)8-10
InchiKey:	ACKNHGGPBUIIMJN-UHFFFAOYSA-N
Formula:	C17H16Cl2O2
SMILES:	CC(C)(C)c1ccc(O)c(C(=O)c2ccc(Cl)c(Cl)c2)c1
Mol. weight [g/mol]:	323.21
CAS:	94622-10-3

Physical Properties

Property code	Value	Unit	Source
gf	-16.37	kJ/mol	Joback Method
hf	-285.68	kJ/mol	Joback Method
hfus	35.06	kJ/mol	Joback Method
hvap	87.21	kJ/mol	Joback Method
log10ws	-5.66		Crippen Method
logp	5.228		Crippen Method
mcvol	234.790	ml/mol	McGowan Method
pc	2320.31	kPa	Joback Method
tb	862.78	K	Joback Method
tc	1119.96	K	Joback Method
tf	595.66	K	Joback Method
vc	0.831	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	640.66	J/molxK	862.78	Joback Method
cpg	653.47	J/molxK	905.64	Joback Method
cpg	665.64	J/molxK	948.51	Joback Method
cpg	677.34	J/molxK	991.37	Joback Method
cpg	688.74	J/molxK	1034.23	Joback Method
cpg	700.05	J/molxK	1077.10	Joback Method
cpg	711.42	J/molxK	1119.96	Joback Method
dvisc	0.0000656	Paxs	595.66	Joback Method
dvisc	0.0000359	Paxs	640.18	Joback Method

dvisc	0.0000212	Paxs	684.70	Joback Method
dvisc	0.0000134	Paxs	729.22	Joback Method
dvisc	0.0000089	Paxs	773.74	Joback Method
dvisc	0.0000062	Paxs	818.26	Joback Method
dvisc	0.0000045	Paxs	862.78	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C94622103&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
mccvol:	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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