

2,4-Ditert-butylphenyl 2,2-dichloropropanoate

Inchi:	InChI=1S/C17H24Cl2O2/c1-15(2,3)11-8-9-13(12(10-11)16(4,5)6)21-14(20)17(7,18)19/h8
InchiKey:	FMBVLXLQSTUNDN-UHFFFAOYSA-N
Formula:	C17H24Cl2O2
SMILES:	CC(Cl)(Cl)C(=O)Oc1ccc(C(C)(C)C)cc1C(C)(C)C
Mol. weight [g/mol]:	331.28
CAS:	116402-58-5

Physical Properties

Property code	Value	Unit	Source
gf	-63.85	kJ/mol	Joback Method
hf	-483.15	kJ/mol	Joback Method
hfus	21.99	kJ/mol	Joback Method
hvap	71.07	kJ/mol	Joback Method
log10ws	-5.74		Crippen Method
logp	5.381		Crippen Method
mcvol	258.550	ml/mol	McGowan Method
pc	1574.70	kPa	Joback Method
tb	766.46	K	Joback Method
tc	997.70	K	Joback Method
tf	472.07	K	Joback Method
vc	0.969	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	718.47	J/molxK	766.46	Joback Method
cpg	788.35	J/molxK	959.16	Joback Method
cpg	776.36	J/molxK	920.62	Joback Method
cpg	763.49	J/molxK	882.08	Joback Method
cpg	749.63	J/molxK	843.54	Joback Method
cpg	734.66	J/molxK	805.00	Joback Method
cpg	799.58	J/molxK	997.70	Joback Method
dvisc	0.0000467	Paxs	766.46	Joback Method
dvisc	0.0000625	Paxs	717.39	Joback Method

dvisc	0.0000874	Paxs	668.33	Joback Method
dvisc	0.0001288	Paxs	619.26	Joback Method
dvisc	0.0002030	Paxs	570.20	Joback Method
dvisc	0.0003487	Paxs	521.13	Joback Method
dvisc	0.0006699	Paxs	472.07	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=C116402585&Units=SI

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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