Phthalic acid, isobutyl 2,4,5-trichlorophenyl ester

Inchi: InChI=1S/C18H15Cl3O4/c1-10(2)9-24-17(22)11-5-3-4-6-12(11)18(23)25-16-8-14(20)13(1

InchiKey: KYVFGNDKBKJZIY-UHFFFAOYSA-N

Formula: C18H15Cl3O4

SMILES: CC(C)COC(=O)c1ccccc1C(=O)Oc1cc(Cl)c(Cl)cc1Cl

Mol. weight [g/mol]: 401.67

Physical Properties

Property code	Value	Unit	Source
gf	-219.09	kJ/mol	Joback Method
hf	-529.77	kJ/mol	Joback Method
hfus	43.54	kJ/mol	Joback Method
hvap	93.94	kJ/mol	Joback Method
log10ws	-6.87		Crippen Method
logp	5.679		Crippen Method
mcvol	268.560	ml/mol	McGowan Method
pc	1803.09	kPa	Joback Method
rinpol	2685.00		NIST Webbook
rinpol	2685.00		NIST Webbook
tb	948.95	K	Joback Method
tc	1191.57	K	Joback Method
tf	614.62	K	Joback Method
vc	1.016	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	727.27	J/mol×K	948.95	Joback Method
cpg	736.84	J/mol×K	989.39	Joback Method
cpg	745.12	J/mol×K	1029.82	Joback Method
cpg	752.13	J/mol×K	1070.26	Joback Method
cpg	757.88	J/mol×K	1110.70	Joback Method
cpg	762.39	J/mol×K	1151.13	Joback Method
cpg	765.69	J/mol×K	1191.57	Joback Method
dvisc	0.0002812	Pa×s	614.62	Joback Method

dvisc	0.0001835	Pa×s	670.34	Joback Method
dvisc	0.0001279	Pa×s	726.06	Joback Method
dvisc	0.0000938	Pa×s	781.79	Joback Method
dvisc	0.0000717	Pa×s	837.51	Joback Method
dvisc	0.0000567	Pa×s	893.23	Joback Method
dvisc	0.0000461	Pa×s	948.95	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357043&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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