Isophthalic acid, butyl 2,4,6-trichlorophenyl ester

Inchi: InChI=1S/C18H15Cl3O4/c1-2-3-7-24-17(22)11-5-4-6-12(8-11)18(23)25-16-14(20)9-13(19

InchiKey: MDZDVLFGORKZCL-UHFFFAOYSA-N

Formula: C18H15Cl3O4

SMILES: CCCCOC(=O)c1cccc(C(=O)Oc2c(Cl)cc(Cl)cc2Cl)c1

Mol. weight [g/mol]: 401.67

Physical Properties

Property code	Value	Unit	Source
gf	-216.65	kJ/mol	Joback Method
hf	-524.49	kJ/mol	Joback Method
hfus	47.07	kJ/mol	Joback Method
hvap	94.33	kJ/mol	Joback Method
log10ws	-7.11		Crippen Method
logp	5.823		Crippen Method
mcvol	268.560	ml/mol	McGowan Method
pc	1790.91	kPa	Joback Method
rinpol	2878.00		NIST Webbook
rinpol	2878.00		NIST Webbook
tb	949.39	K	Joback Method
tc	1189.09	K	Joback Method
tf	629.62	K	Joback Method
vc	1.022	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	726.75	J/mol×K	949.39	Joback Method
cpg	762.06	J/mol×K	1149.14	Joback Method
cpg	757.42	J/mol×K	1109.19	Joback Method
cpg	751.59	J/mol×K	1069.24	Joback Method
cpg	744.55	J/mol×K	1029.29	Joback Method
cpg	736.27	J/mol×K	989.34	Joback Method
cpg	765.53	J/mol×K	1189.09	Joback Method
dvisc	0.0000506	Pa×s	949.39	Joback Method

dvisc	0.0000615	Pa×s	896.09	Joback Method
dvisc	0.0000766	Pa×s	842.80	Joback Method
dvisc	0.0000983	Pa×s	789.50	Joback Method
dvisc	0.0001308	Pa×s	736.21	Joback Method
dvisc	0.0001821	Pa×s	682.91	Joback Method
dvisc	0.0002679	Pa×s	629.62	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U344568&Units=SI
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

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