

Phthalic acid, butyl 3,4,5-trichlorophenyl ester

Inchi:	InChI=1S/C18H15Cl3O4/c1-2-3-8-24-17(22)12-6-4-5-7-13(12)18(23)25-11-9-14(19)16(2)
InchiKey:	DHLVFOXDYPMTMO-UHFFFAOYSA-N
Formula:	C18H15Cl3O4
SMILES:	CCCCOC(=O)c1ccccc1C(=O)Oc1cc(Cl)c(Cl)c(Cl)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
rinsol	2788.00		NIST Webbook
tb	949.39	K	Joback Method
tc	1189.09	K	Joback Method
tf	629.62	K	Joback Method
vc	1.022	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	726.75	J/molxK	949.39	Joback Method
cpg	736.27	J/molxK	989.34	Joback Method
cpg	744.55	J/molxK	1029.29	Joback Method
cpg	751.59	J/molxK	1069.24	Joback Method
cpg	757.42	J/molxK	1109.19	Joback Method
cpg	762.06	J/molxK	1149.14	Joback Method
cpg	765.53	J/molxK	1189.09	Joback Method
dvisc	0.0002679	Paxs	629.62	Joback Method
dvisc	0.0001821	Paxs	682.91	Joback Method

dvisc	0.0001308	Paxs	736.21	Joback Method
dvisc	0.0000983	Paxs	789.50	Joback Method
dvisc	0.0000766	Paxs	842.80	Joback Method
dvisc	0.0000615	Paxs	896.09	Joback Method
dvisc	0.0000506	Paxs	949.39	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=U357066&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
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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