Phthalic acid, 2,5-dichlorophenyl isobutyl ester

Inchi: InChI=1S/C18H16Cl2O4/c1-11(2)10-23-17(21)13-5-3-4-6-14(13)18(22)24-16-9-12(19)7-8

InchiKey: STAZZNAMXXZGHF-UHFFFAOYSA-N

Formula: C18H16Cl2O4

SMILES: CC(C)COC(=O)c1ccccc1C(=O)Oc1cc(Cl)ccc1Cl

Mol. weight [g/mol]: 367.22

Physical Properties

Property code	Value	Unit	Source
gf	-197.53	kJ/mol	Joback Method
hf	-502.56	kJ/mol	Joback Method
hfus	39.74	kJ/mol	Joback Method
hvap	88.89	kJ/mol	Joback Method
log10ws	-6.19		Crippen Method
logp	5.025		Crippen Method
mcvol	256.320	ml/mol	McGowan Method
pc	1885.44	kPa	Joback Method
rinpol	2512.00		NIST Webbook
rinpol	2512.00		NIST Webbook
tb	906.54	K	Joback Method
tc	1145.54	K	Joback Method
tf	572.18	K	Joback Method
vc	0.968	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	709.90	J/mol×K	906.54	Joback Method
cpg	721.00	J/mol×K	946.37	Joback Method
cpg	730.81	J/mol×K	986.21	Joback Method
cpg	739.36	J/mol×K	1026.04	Joback Method
cpg	746.68	J/mol×K	1065.87	Joback Method
cpg	752.79	J/mol×K	1105.71	Joback Method
cpg	757.72	J/mol×K	1145.54	Joback Method
dvisc	0.0003726	Pa×s	572.18	Joback Method

dvisc	0.0002327	Pa×s	627.91	Joback Method
dvisc	0.0001569	Pa×s	683.63	Joback Method
dvisc	0.0001123	Pa×s	739.36	Joback Method
dvisc	0.0000842	Pa×s	795.09	Joback Method
dvisc	0.0000656	Pa×s	850.81	Joback Method
dvisc	0.0000527	Pa×s	906.54	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=U356376&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

Latest version available from:
https://www.chemeo.com/cid/55-949-8/Phthalic-acid-2-5-dichlorophenyl-isobutyl-ester.pdf
Generated by Cheméo on 2024-04-26 17:39:19.819464907 +0000 UTC m=+16442408.740042217.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.