Phthalic acid, butyl 2,5-dichlorophenyl ester

Inchi: InChI=1S/C18H16Cl2O4/c1-2-3-10-23-17(21)13-6-4-5-7-14(13)18(22)24-16-11-12(19)8-9
InchiKey: PYDBQZXFMVMSGK-UHFFFAOYSA-N
Formula: C18H16Cl2O4
SMILES: CCCCOC(=O)c1ccccc1C(=O)Oc1cc(Cl)ccc1Cl
Mol. weight [g/mol]: 367.22

Physical Properties

Property code	Value	Unit	Source
gf	-195.09	kJ/mol	Joback Method
hf	-497.28	kJ/mol	Joback Method
hfus	43.26	kJ/mol	Joback Method
hvap	89.28	kJ/mol	Joback Method
log10ws	-6.43		Crippen Method
logp	5.170		Crippen Method
mcvol	256.320	ml/mol	McGowan Method
pc	1872.41	kPa	Joback Method
rinpol	2568.00		NIST Webbook
rinpol	2568.00		NIST Webbook
tb	906.98	K	Joback Method
tc	1142.81	K	Joback Method
tf	587.18	K	Joback Method
vc	0.974	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	709.35	J/mol×K	906.98	Joback Method
cpg	720.35	J/mol×K	946.28	Joback Method
cpg	730.10	J/mol×K	985.59	Joback Method
cpg	738.64	J/mol×K	1024.89	Joback Method
cpg	746.00	J/mol×K	1064.20	Joback Method
cpg	752.20	J/mol×K	1103.50	Joback Method
cpg	757.26	J/mol×K	1142.81	Joback Method
dvisc	0.0003488	Pa×s	587.18	Joback Method

dvisc	0.0002281	Pa×s	640.48	Joback Method
dvisc	0.0001592	Pa×s	693.78	Joback Method
dvisc	0.0001170	Pa×s	747.08	Joback Method
dvisc	0.0000895	Pa×s	800.38	Joback Method
dvisc	0.0000709	Pa×s	853.68	Joback Method
dvisc	0.0000577	Pa×s	906.98	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=U356375&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