Isophthalic acid, 3,5-dichlorophenyl pentyl ester

Inchi: InChI=1S/C19H18Cl2O4/c1-2-3-4-8-24-18(22)13-6-5-7-14(9-13)19(23)25-17-11-15(20)1(

InchiKey: MIKBGKKSTZJFAQ-UHFFFAOYSA-N

Formula: C19H18Cl2O4

SMILES: CCCCCOC(=O)c1cccc(C(=O)Oc2cc(Cl)cc(Cl)c2)c1

Mol. weight [g/mol]: 381.25

Physical Properties

Property code	Value	Unit	Source
gf	-186.67	kJ/mol	Joback Method
hf	-517.92	kJ/mol	Joback Method
hfus	45.85	kJ/mol	Joback Method
hvap	91.51	kJ/mol	Joback Method
log10ws	-6.85		Crippen Method
logp	5.560		Crippen Method
mcvol	270.410	ml/mol	McGowan Method
pc	1726.03	kPa	Joback Method
rinpol	2823.00		NIST Webbook
tb	929.86	K	Joback Method
tc	1163.73	K	Joback Method
tf	598.45	K	Joback Method
vc	1.030	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	765.86	J/mol×K	929.86	Joback Method
cpg	776.98	J/mol×K	968.84	Joback Method
cpg	786.84	J/mol×K	1007.82	Joback Method
cpg	795.46	J/mol×K	1046.79	Joback Method
cpg	802.88	J/mol×K	1085.77	Joback Method
cpg	809.13	J/mol×K	1124.75	Joback Method
cpg	814.22	J/mol×K	1163.73	Joback Method
dvisc	0.0003155	Pa×s	598.45	Joback Method
dvisc	0.0002039	Pa×s	653.69	Joback Method

dvisc	0.0001411	Pa×s	708.92	Joback Method
dvisc	0.0001029	Pa×s	764.15	Joback Method
dvisc	0.0000784	Pa×s	819.39	Joback Method
dvisc	0.0000617	Pa×s	874.62	Joback Method
dvisc	0.0000500	Pa×s	929.86	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=U356583&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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