Isophthalic acid, pentyl 2,3,5-trichlorophenyl ester

Inchi: InChI=1S/C19H17Cl3O4/c1-2-3-4-8-25-18(23)12-6-5-7-13(9-12)19(24)26-16-11-14(20)10

InchiKey: RNGGSFNLFQLBGO-UHFFFAOYSA-N

Formula: C19H17Cl3O4

SMILES: CCCCCOC(=O)c1cccc(C(=O)Oc2cc(Cl)cc(Cl)c2Cl)c1

Mol. weight [g/mol]: 415.69

Physical Properties

Property code	Value	Unit	Source
gf	-208.23	kJ/mol	Joback Method
hf	-545.13	kJ/mol	Joback Method
hfus	49.66	kJ/mol	Joback Method
hvap	96.55	kJ/mol	Joback Method
log10ws	-7.53		Crippen Method
logp	6.213		Crippen Method
mcvol	282.650	ml/mol	McGowan Method
pc	1653.80	kPa	Joback Method
rinpol	2972.00		NIST Webbook
rinpol	2972.00		NIST Webbook
tb	972.27	K	Joback Method
tc	1210.51	K	Joback Method
tf	640.89	K	Joback Method
vc	1.079	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	783.33	J/mol×K	972.27	Joback Method
cpg	792.96	J/mol×K	1011.98	Joback Method
cpg	801.32	J/mol×K	1051.68	Joback Method
cpg	808.41	J/mol×K	1091.39	Joback Method
cpg	814.28	J/mol×K	1131.10	Joback Method
cpg	818.93	J/mol×K	1170.81	Joback Method
cpg	822.41	J/mol×K	1210.51	Joback Method
dvisc	0.0002413	Pa×s	640.89	Joback Method

dvisc	0.0001621	Pa×s	696.12	Joback Method
dvisc	0.0001155	Pa×s	751.35	Joback Method
dvisc	0.0000862	Pa×s	806.58	Joback Method
dvisc	0.0000668	Pa×s	861.81	Joback Method
dvisc	0.0000533	Pa×s	917.04	Joback Method
dvisc	0.0000437	Pa×s	972.27	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=U356620&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