

Isophthalic acid, pentyl 2,4,6-trichlorophenyl ester

Inchi:	InChI=1S/C19H17Cl3O4/c1-2-3-4-8-25-18(23)12-6-5-7-13(9-12)19(24)26-17-15(21)10-14
InchiKey:	ORONDZAYKDKYQE-UHFFFAOYSA-N
Formula:	C19H17Cl3O4
SMILES:	CCCCCOC(=O)c1cccc(C(=O)Oc2c(Cl)cc(Cl)cc2Cl)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	2994.00		NIST Webbook
rinpol	2994.00		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/molxK	972.27	Joback Method
cpg	792.96	J/molxK	1011.98	Joback Method
cpg	801.32	J/molxK	1051.68	Joback Method
cpg	808.41	J/molxK	1091.39	Joback Method
cpg	814.28	J/molxK	1131.10	Joback Method
cpg	818.93	J/molxK	1170.81	Joback Method
cpg	822.41	J/molxK	1210.51	Joback Method
dvisc	0.0002413	Paxs	640.89	Joback Method

dvisc	0.0001621	Paxs	696.12	Joback Method
dvisc	0.0001155	Paxs	751.35	Joback Method
dvisc	0.0000862	Paxs	806.58	Joback Method
dvisc	0.0000668	Paxs	861.81	Joback Method
dvisc	0.0000533	Paxs	917.04	Joback Method
dvisc	0.0000437	Paxs	972.27	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U344569&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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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