

Phthalic acid, di(2,3,5-trichlorophenyl) ester

Inchi: InChI=1S/C20H8Cl6O4/c21-9-5-13(23)17(25)15(7-9)29-19(27)11-3-1-2-4-12(11)20(28)30
InchiKey: OCTZGBNMQULYIY-UHFFFAOYSA-N
Formula: C20H8Cl6O4
SMILES: O=C(Oc1cc(Cl)cc(Cl)c1Cl)c1ccccc1C(=O)Oc1cc(Cl)cc(Cl)c1Cl
Mol. weight [g/mol]: 524.99

Physical Properties

Property code	Value	Unit	Source
gf	-152.08	kJ/mol	Joback Method
hf	-410.87	kJ/mol	Joback Method
hfus	57.71	kJ/mol	Joback Method
hvap	116.20	kJ/mol	Joback Method
log10ws	-9.76		Crippen Method
logp	8.045		Crippen Method
mcvol	309.700	ml/mol	McGowan Method
pc	1765.41	kPa	Joback Method
rinpol	3530.00		NIST Webbook
rinpol	3530.00		NIST Webbook
tb	1149.06	K	Joback Method
tc	1424.67	K	Joback Method
tf	805.90	K	Joback Method
vc	1.173	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	756.19	J/molxK	1149.06	Joback Method
cpg	751.76	J/molxK	1378.74	Joback Method
cpg	755.50	J/molxK	1332.80	Joback Method
cpg	757.85	J/molxK	1286.87	Joback Method
cpg	758.76	J/molxK	1240.93	Joback Method
cpg	758.22	J/molxK	1195.00	Joback Method
cpg	746.66	J/molxK	1424.67	Joback Method
dvisc	0.0000257	Paxs	1149.06	Joback Method

dvisc	0.0000304	Paxs	1091.87	Joback Method
dvisc	0.0000366	Paxs	1034.67	Joback Method
dvisc	0.0000451	Paxs	977.48	Joback Method
dvisc	0.0000571	Paxs	920.29	Joback Method
dvisc	0.0000745	Paxs	863.09	Joback Method
dvisc	0.0001010	Paxs	805.90	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357062&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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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