

Phthalic acid, isoheptyl 3,4,5-trichlorophenyl ester

Inchi:	InChI=1S/C20H19Cl3O4/c1-12(2)6-5-9-26-19(24)14-7-3-4-8-15(14)20(25)27-13-10-16(2)
InchiKey:	RHFDMLPOUCGTNX-UHFFFAOYSA-N
Formula:	C20H19Cl3O4
SMILES:	CC(C)CCCOC(=O)c1ccccc1C(=O)Oc1cc(Cl)c(Cl)c(Cl)c1
Mol. weight [g/mol]:	429.72

Physical Properties

Property code	Value	Unit	Source
gf	-202.25	kJ/mol	Joback Method
hf	-571.05	kJ/mol	Joback Method
hfus	48.72	kJ/mol	Joback Method
hvap	98.39	kJ/mol	Joback Method
log10ws	-7.71		Crippen Method
logp	6.459		Crippen Method
mcvol	296.740	ml/mol	McGowan Method
pc	1541.49	kPa	Joback Method
rinpol	2931.00		NIST Webbook
rinpol	2931.00		NIST Webbook
tb	994.71	K	Joback Method
tc	1234.50	K	Joback Method
tf	637.16	K	Joback Method
vc	1.129	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	840.96	J/molxK	994.71	Joback Method
cpg	876.35	J/molxK	1194.53	Joback Method
cpg	871.87	J/molxK	1154.57	Joback Method
cpg	866.11	J/molxK	1114.60	Joback Method
cpg	859.06	J/molxK	1074.64	Joback Method
cpg	850.69	J/molxK	1034.67	Joback Method
cpg	879.60	J/molxK	1234.50	Joback Method
dvisc	0.0000343	Paxs	994.71	Joback Method

dvisc	0.0000425	Paxs	935.12	Joback Method
dvisc	0.0000543	Paxs	875.53	Joback Method
dvisc	0.0000717	Paxs	815.93	Joback Method
dvisc	0.0000991	Paxs	756.34	Joback Method
dvisc	0.0001446	Paxs	696.75	Joback Method
dvisc	0.0002265	Paxs	637.16	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357068&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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