

Phthalic acid, nonyl 2,4,6-trichlorobenzyl ester

Inchi:	InChI=1S/C24H27Cl3O4/c1-2-3-4-5-6-7-10-13-30-23(28)18-11-8-9-12-19(18)24(29)31-16
InchiKey:	MBKRMIURVPUAPY-UHFFFAOYSA-N
Formula:	C24H27Cl3O4
SMILES:	CCCCCCCCCOC(=O)c1ccccc1C(=O)OCc1c(Cl)cc(Cl)cc1Cl
Mol. weight [g/mol]:	485.83

Physical Properties

Property code	Value	Unit	Source
gf	-166.13	kJ/mol	Joback Method
hf	-648.33	kJ/mol	Joback Method
hfus	62.61	kJ/mol	Joback Method
hvap	107.68	kJ/mol	Joback Method
log10ws	-9.47		Crippen Method
logp	7.911		Crippen Method
mcvol	353.100	ml/mol	McGowan Method
pc	1157.71	kPa	Joback Method
rinpol	3256.00		NIST Webbook
rinpol	3256.00		NIST Webbook
tb	1086.67	K	Joback Method
tc	1331.19	K	Joback Method
tf	697.24	K	Joback Method
vc	1.359	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1074.42	J/molxK	1086.67	Joback Method
cpg	1084.30	J/molxK	1127.42	Joback Method
cpg	1092.67	J/molxK	1168.18	Joback Method
cpg	1099.58	J/molxK	1208.93	Joback Method
cpg	1105.09	J/molxK	1249.68	Joback Method
cpg	1109.23	J/molxK	1290.44	Joback Method
cpg	1112.07	J/molxK	1331.19	Joback Method
dvisc	0.0001366	Paxs	697.24	Joback Method

dvisc	0.0000871	Paxs	762.14	Joback Method
dvisc	0.0000596	Paxs	827.05	Joback Method
dvisc	0.0000431	Paxs	891.96	Joback Method
dvisc	0.0000326	Paxs	956.86	Joback Method
dvisc	0.0000255	Paxs	1021.77	Joback Method
dvisc	0.0000206	Paxs	1086.67	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382883&Units=SI
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

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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