

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

Inchi:	InChI=1S/C20H19Cl3O4/c1-2-3-6-9-26-19(24)14-7-4-5-8-15(14)20(25)27-12-16-17(22)10
InchiKey:	IPSAOAQQNQPMPLP-UHFFFAOYSA-N
Formula:	C20H19Cl3O4
SMILES:	CCCCCOC(=O)c1cccc1C(=O)OCc1c(Cl)cc(Cl)cc1Cl
Mol. weight [g/mol]:	429.72

Physical Properties

Property code	Value	Unit	Source
gf	-199.81	kJ/mol	Joback Method
hf	-565.77	kJ/mol	Joback Method
hfus	52.25	kJ/mol	Joback Method
hvap	98.78	kJ/mol	Joback Method
log10ws	-7.80		Crippen Method
logp	6.351		Crippen Method
mcvol	296.740	ml/mol	McGowan Method
pc	1531.86	kPa	Joback Method
rinpol	2861.00		NIST Webbook
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tb	995.15	K	Joback Method
tc	1232.78	K	Joback Method
tf	652.16	K	Joback Method
vc	1.135	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	840.52	J/molxK	995.15	Joback Method
cpg	876.24	J/molxK	1193.17	Joback Method
cpg	871.62	J/molxK	1153.57	Joback Method
cpg	865.76	J/molxK	1113.96	Joback Method
cpg	858.64	J/molxK	1074.36	Joback Method
cpg	850.24	J/molxK	1034.75	Joback Method
cpg	879.67	J/molxK	1232.78	Joback Method
dvisc	0.0000377	Paxs	995.15	Joback Method

dvisc	0.0000462	Paxs	937.98	Joback Method
dvisc	0.0000581	Paxs	880.82	Joback Method
dvisc	0.0000754	Paxs	823.65	Joback Method
dvisc	0.0001017	Paxs	766.49	Joback Method
dvisc	0.0001439	Paxs	709.32	Joback Method
dvisc	0.0002166	Paxs	652.16	Joback Method

Sources

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=U382879&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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