

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

Inchi:	InChI=1S/C21H21Cl3O4/c1-2-3-4-7-10-27-20(25)15-8-5-6-9-16(15)21(26)28-13-17-18(2)
InchiKey:	QKMNJCQRSJMPY-UHFFFAOYSA-N
Formula:	C21H21Cl3O4
SMILES:	CCCCCOC(=O)c1cccc1C(=O)OCc1c(Cl)cc(Cl)cc1Cl
Mol. weight [g/mol]:	443.75

Physical Properties

Property code	Value	Unit	Source
gf	-191.39	kJ/mol	Joback Method
hf	-586.41	kJ/mol	Joback Method
hfus	54.84	kJ/mol	Joback Method
hvap	101.01	kJ/mol	Joback Method
log10ws	-8.21		Crippen Method
logp	6.741		Crippen Method
mvol	310.830	ml/mol	McGowan Method
pc	1422.92	kPa	Joback Method
rinpol	2958.00		NIST Webbook
rinpol	2958.00		NIST Webbook
tb	1018.03	K	Joback Method
tc	1255.93	K	Joback Method
tf	663.43	K	Joback Method
vc	1.190	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	898.28	J/molxK	1018.03	Joback Method
cpg	933.96	J/molxK	1216.28	Joback Method
cpg	929.40	J/molxK	1176.63	Joback Method
cpg	923.58	J/molxK	1136.98	Joback Method
cpg	916.48	J/molxK	1097.33	Joback Method
cpg	908.06	J/molxK	1057.68	Joback Method
cpg	937.30	J/molxK	1255.93	Joback Method
dvisc	0.0000325	Paxs	1018.03	Joback Method

dvisc	0.0000399	Paxs	958.93	Joback Method
dvisc	0.0000504	Paxs	899.83	Joback Method
dvisc	0.0000658	Paxs	840.73	Joback Method
dvisc	0.0000893	Paxs	781.63	Joback Method
dvisc	0.0001274	Paxs	722.53	Joback Method
dvisc	0.0001938	Paxs	663.43	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382880&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

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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