

Phthalic acid, 4-chloro-2-methoxybenzyl pentyl ester

Inchi:	InChI=1S/C21H23ClO5/c1-3-4-7-12-26-20(23)17-8-5-6-9-18(17)21(24)27-14-15-10-11-16
InchiKey:	DATWLYOYGGJGFA-UHFFFAOYSA-N
Formula:	C21H23ClO5
SMILES:	CCCCCOC(=O)c1cccc1C(=O)OCc1ccc(Cl)cc1OC
Mol. weight [g/mol]:	390.86

Physical Properties

Property code	Value	Unit	Source
gf	-262.90	kJ/mol	Joback Method
hf	-675.68	kJ/mol	Joback Method
hfus	48.02	kJ/mol	Joback Method
hvap	93.98	kJ/mol	Joback Method
log10ws	-6.55		Crippen Method
logp	5.053		Crippen Method
mvol	292.220	ml/mol	McGowan Method
pc	1503.48	kPa	Joback Method
rinpol	2777.00		NIST Webbook
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tb	960.61	K	Joback Method
tc	1188.92	K	Joback Method
tf	613.30	K	Joback Method
vc	1.111	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	886.22	J/molxK	960.61	Joback Method
cpg	930.55	J/molxK	1150.87	Joback Method
cpg	924.55	J/molxK	1112.82	Joback Method
cpg	917.14	J/molxK	1074.76	Joback Method
cpg	908.29	J/molxK	1036.71	Joback Method
cpg	897.99	J/molxK	998.66	Joback Method
cpg	935.13	J/molxK	1188.92	Joback Method
dvisc	0.0000327	Paxs	960.61	Joback Method

dvisc	0.0000405	Paxs	902.72	Joback Method
dvisc	0.0000518	Paxs	844.84	Joback Method
dvisc	0.0000686	Paxs	786.95	Joback Method
dvisc	0.0000950	Paxs	729.07	Joback Method
dvisc	0.0001393	Paxs	671.19	Joback Method
dvisc	0.0002194	Paxs	613.30	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=U382839&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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