

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

Inchi:	InChI=1S/C22H25ClO5/c1-3-4-5-8-13-27-21(24)18-9-6-7-10-19(18)22(25)28-15-16-11-12
InchiKey:	CYTFQPPEXZHLR-UHFFFAOYSA-N
Formula:	C22H25ClO5
SMILES:	CCCCCCOC(=O)c1ccccc1C(=O)OCc1ccc(Cl)cc1OC
Mol. weight [g/mol]:	404.88

Physical Properties

Property code	Value	Unit	Source
gf	-254.48	kJ/mol	Joback Method
hf	-696.32	kJ/mol	Joback Method
hfus	50.61	kJ/mol	Joback Method
hvap	96.21	kJ/mol	Joback Method
log10ws	-6.96		Crippen Method
logp	5.443		Crippen Method
mvol	306.310	ml/mol	McGowan Method
pc	1397.50	kPa	Joback Method
rinpol	2878.00		NIST Webbook
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tb	983.49	K	Joback Method
tc	1212.44	K	Joback Method
tf	624.57	K	Joback Method
vc	1.167	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	944.70	J/molxK	983.49	Joback Method
cpg	956.44	J/molxK	1021.65	Joback Method
cpg	966.67	J/molxK	1059.81	Joback Method
cpg	975.40	J/molxK	1097.96	Joback Method
cpg	982.65	J/molxK	1136.12	Joback Method
cpg	988.44	J/molxK	1174.28	Joback Method
cpg	992.78	J/molxK	1212.44	Joback Method
dvisc	0.0001969	Paxs	624.57	Joback Method

dvisc	0.0001236	Paxs	684.39	Joback Method
dvisc	0.0000837	Paxs	744.21	Joback Method
dvisc	0.0000600	Paxs	804.03	Joback Method
dvisc	0.0000451	Paxs	863.85	Joback Method
dvisc	0.0000351	Paxs	923.67	Joback Method
dvisc	0.0000282	Paxs	983.49	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382840&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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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