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

Inchi: InChI=1S/C23H27ClO5/c1-3-4-5-6-9-14-28-22(25)19-10-7-8-11-20(19)23(26)29-16-17-12

InchiKey: FKKGXVMJFKCROB-UHFFFAOYSA-N

Formula: C23H27ClO5

SMILES: CCCCCCCOC(=O)c1ccccc1C(=O)OCc1ccc(Cl)cc1OC

Mol. weight [g/mol]: 418.91

Physical Properties

Property code	Value	Unit	Source
gf	-246.06	kJ/mol	Joback Method
hf	-716.96	kJ/mol	Joback Method
hfus	53.20	kJ/mol	Joback Method
hvap	98.44	kJ/mol	Joback Method
log10ws	-7.38		Crippen Method
logp	5.833		Crippen Method
mcvol	320.400	ml/mol	McGowan Method
pc	1302.35	kPa	Joback Method
rinpol	2973.00		NIST Webbook
rinpol	2973.00		NIST Webbook
tb	1006.37	K	Joback Method
tc	1236.86	K	Joback Method
tf	635.84	K	Joback Method
vc	1.222	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1003.65	J/mol×K	1006.37	Joback Method
cpg	1015.36	J/mol×K	1044.79	Joback Method
cpg	1025.49	J/mol×K	1083.20	Joback Method
cpg	1034.07	J/mol×K	1121.62	Joback Method
cpg	1041.11	J/mol×K	1160.03	Joback Method
cpg	1046.65	J/mol×K	1198.45	Joback Method
cpg	1050.70	J/mol×K	1236.86	Joback Method
dvisc	0.0001762	Pa×s	635.84	Joback Method

dvisc	0.0001095	Pa×s	697.60	Joback Method
dvisc	0.0000735	Pa×s	759.35	Joback Method
dvisc	0.0000524	Pa×s	821.11	Joback Method
dvisc	0.0000391	Pa×s	882.86	Joback Method
dvisc	0.0000304	Pa×s	944.62	Joback Method
dvisc	0.0000243	Pa×s	1006.37	Joback Method

Sources

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=U382841&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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