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

Inchi: InChI=1S/C24H29ClO5/c1-3-4-5-6-7-10-15-29-23(26)20-11-8-9-12-21(20)24(27)30-17-18

InchiKey: KMBAUBTYCMIFGQ-UHFFFAOYSA-N

Formula: C24H29ClO5

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

Mol. weight [g/mol]: 432.94

Physical Properties

Property code	Value	Unit	Source
gf	-237.64	kJ/mol	Joback Method
hf	-737.60	kJ/mol	Joback Method
hfus	55.79	kJ/mol	Joback Method
hvap	100.66	kJ/mol	Joback Method
log10ws	-7.80		Crippen Method
logp	6.223		Crippen Method
mcvol	334.490	ml/mol	McGowan Method
pc	1216.59	kPa	Joback Method
rinpol	3071.00		NIST Webbook
rinpol	3071.00		NIST Webbook
tb	1029.25	K	Joback Method
tc	1262.24	K	Joback Method
tf	647.11	K	Joback Method
vc	1.278	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1063.03	J/mol×K	1029.25	Joback Method
cpg	1105.13	J/mol×K	1223.41	Joback Method
cpg	1099.89	J/mol×K	1184.58	Joback Method
cpg	1093.09	J/mol×K	1145.75	Joback Method
cpg	1084.70	J/mol×K	1106.91	Joback Method
cpg	1074.69	J/mol×K	1068.08	Joback Method
cpg	1108.83	J/mol×K	1262.24	Joback Method
dvisc	0.0000209	Pa×s	1029.25	Joback Method

dvisc	0.0000262	Pa×s	965.56	Joback Method
dvisc	0.0000339	Pa×s	901.87	Joback Method
dvisc	0.0000456	Pa×s	838.18	Joback Method
dvisc	0.0000644	Pa×s	774.49	Joback Method
dvisc	0.0000966	Pa×s	710.80	Joback Method
dvisc	0.0001572	Pa×s	647.11	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=U382842&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