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

Inchi: InChI=1S/C25H31ClO5/c1-3-4-5-6-7-8-11-16-30-24(27)21-12-9-10-13-22(21)25(28)31-18

InchiKey: CIIGJJAPZYFGLR-UHFFFAOYSA-N

Formula: C25H31ClO5

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

Mol. weight [g/mol]: 446.96

Physical Properties

Property code	Value	Unit	Source
gf	-229.22	kJ/mol	Joback Method
hf	-758.24	kJ/mol	Joback Method
hfus	58.38	kJ/mol	Joback Method
hvap	102.89	kJ/mol	Joback Method
log10ws	-8.22		Crippen Method
logp	6.613		Crippen Method
mcvol	348.580	ml/mol	McGowan Method
pc	1139.03	kPa	Joback Method
rinpol	3172.00		NIST Webbook
rinpol	3172.00		NIST Webbook
tb	1052.13	K	Joback Method
tc	1288.64	K	Joback Method
tf	658.38	K	Joback Method
vc	1.335	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1122.78	J/mol×K	1052.13	Joback Method
cpg	1163.83	J/mol×K	1249.22	Joback Method
cpg	1158.94	J/mol×K	1209.80	Joback Method
cpg	1152.43	J/mol×K	1170.38	Joback Method
cpg	1144.25	J/mol×K	1130.97	Joback Method
cpg	1134.38	J/mol×K	1091.55	Joback Method
cpg	1167.12	J/mol×K	1288.64	Joback Method
dvisc	0.0000180	Pa×s	1052.13	Joback Method

dvisc	0.0000226	Pa×s	986.50	Joback Method
dvisc	0.0000293	Pa×s	920.88	Joback Method
dvisc	0.0000396	Pa×s	855.25	Joback Method
dvisc	0.0000562	Pa×s	789.63	Joback Method
dvisc	0.0000851	Pa×s	724.01	Joback Method
dvisc	0.0001398	Pa×s	658.38	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382843&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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