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

Inchi: InChI=1S/C26H33ClO5/c1-3-4-5-6-7-8-9-12-17-31-25(28)22-13-10-11-14-23(22)26(29)32

InchiKey: LSYYJKBKFHCQEV-UHFFFAOYSA-N

Formula: C26H33ClO5

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

Mol. weight [g/mol]: 460.99

Physical Properties

Property code	Value	Unit	Source
gf	-220.80	kJ/mol	Joback Method
hf	-778.88	kJ/mol	Joback Method
hfus	60.97	kJ/mol	Joback Method
hvap	105.11	kJ/mol	Joback Method
log10ws	-8.64		Crippen Method
logp	7.003		Crippen Method
mcvol	362.670	ml/mol	McGowan Method
pc	1068.66	kPa	Joback Method
rinpol	3270.00		NIST Webbook
rinpol	3270.00		NIST Webbook
tb	1075.01	K	Joback Method
tc	1316.11	K	Joback Method
tf	669.65	K	Joback Method
vc	1.391	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1182.86	J/mol×K	1075.01	Joback Method
cpg	1194.39	J/mol×K	1115.19	Joback Method
cpg	1204.10	J/mol×K	1155.38	Joback Method
cpg	1212.03	J/mol×K	1195.56	Joback Method
cpg	1218.21	J/mol×K	1235.75	Joback Method
cpg	1222.69	J/mol×K	1275.93	Joback Method
cpg	1225.51	J/mol×K	1316.11	Joback Method
dvisc	0.0001240	Pa×s	669.65	Joback Method

dvisc	0.0000747	Pa×s	737.21	Joback Method
dvisc	0.0000490	Pa×s	804.77	Joback Method
dvisc	0.0000343	Pa×s	872.33	Joback Method
dvisc	0.0000253	Pa×s	939.89	Joback Method
dvisc	0.0000194	Pa×s	1007.45	Joback Method
dvisc	0.0000154	Pa×s	1075.01	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382844&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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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