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

Inchi: InChI=1S/C20H21ClO5/c1-3-4-11-25-19(22)16-7-5-6-8-17(16)20(23)26-13-14-9-10-15(21

InchiKey: TYAMFYZWYVZNMV-UHFFFAOYSA-N

Formula: C20H21ClO5

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

Mol. weight [g/mol]: 376.83

Physical Properties

Property code	Value	Unit	Source
gf	-271.32	kJ/mol	Joback Method
hf	-655.04	kJ/mol	Joback Method
hfus	45.43	kJ/mol	Joback Method
hvap	91.76	kJ/mol	Joback Method
log10ws	-6.13		Crippen Method
logp	4.662		Crippen Method
mcvol	278.130	ml/mol	McGowan Method
pc	1621.98	kPa	Joback Method
rinpol	2679.00		NIST Webbook
rinpol	2679.00		NIST Webbook
tb	937.73	K	Joback Method
tc	1166.24	K	Joback Method
tf	602.03	K	Joback Method
vc	1.054	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	828.29	J/mol×K	937.73	Joback Method
cpg	840.05	J/mol×K	975.82	Joback Method
cpg	850.40	J/mol×K	1013.90	Joback Method
cpg	859.33	J/mol×K	1051.99	Joback Method
cpg	866.87	J/mol×K	1090.07	Joback Method
cpg	873.03	J/mol×K	1128.16	Joback Method
cpg	877.80	J/mol×K	1166.24	Joback Method
dvisc	0.0002436	Pa×s	602.03	Joback Method

dvisc	0.0001564	Pa×s	657.98	Joback Method
dvisc	0.0001076	Pa×s	713.93	Joback Method
dvisc	0.0000782	Pa×s	769.88	Joback Method
dvisc	0.0000594	Pa×s	825.83	Joback Method
dvisc	0.0000466	Pa×s	881.78	Joback Method
dvisc	0.0000377	Pa×s	937.73	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=U382838&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