Phthalic acid, dodecyl 3-methoxybenzyl ester

Inchi: InChI=1S/C28H38O5/c1-3-4-5-6-7-8-9-10-11-14-20-32-27(29)25-18-12-13-19-26(25)28(3
InchiKey: UBDLVSVMUXWUDY-UHFFFAOYSA-N
Formula: C28H38O5
SMILES: CCCCCCCCCCCCOC(=O)c1ccccc1C(=O)OCc1cccc(OC)c1
Mol. weight [g/mol]: 454.60

Physical Properties

Property code	Value	Unit	Source
gf	-182.40	kJ/mol	Joback Method
hf	-792.95	kJ/mol	Joback Method
hfus	62.34	kJ/mol	Joback Method
hvap	104.52	kJ/mol	Joback Method
log10ws	-8.79		Crippen Method
logp	7.130		Crippen Method
mcvol	378.610	ml/mol	McGowan Method
pc	977.17	kPa	Joback Method
rinpol	3407.00		NIST Webbook
tb	1078.36	K	Joback Method
tc	1320.98	K	Joback Method
tf	649.75	K	Joback Method
vc	1.454	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1285.63	J/mol×K	1078.36	Joback Method
cpg	1298.89	J/mol×K	1118.80	Joback Method
cpg	1310.23	J/mol×K	1159.23	Joback Method
cpg	1319.72	J/mol×K	1199.67	Joback Method
cpg	1327.41	J/mol×K	1240.10	Joback Method
cpg	1333.35	J/mol×K	1280.54	Joback Method
cpg	1337.60	J/mol×K	1320.98	Joback Method
dvisc	0.0001320	Pa×s	649.75	Joback Method
dvisc	0.0000743	Pa×s	721.19	Joback Method

dvisc	0.0000464	Pa×s	792.62	Joback Method
dvisc	0.0000313	Pa×s	864.06	Joback Method
dvisc	0.0000224	Pa×s	935.49	Joback Method
dvisc	0.0000169	Pa×s	1006.93	Joback Method
dvisc	0.0000132	Pa×s	1078.36	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U377985&Units=SI

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