Phthalic acid, 2-methoxybenzyl nonyl ester

Inchi: InChI=1S/C25H32O5/c1-3-4-5-6-7-8-13-18-29-24(26)21-15-10-11-16-22(21)25(27)30-19
InchiKey: OBPIQTAPJZVCRQ-UHFFFAOYSA-N
Formula: C25H32O5
SMILES: CCCCCCCCCOC(=O)c1ccccc1C(=O)OCc1ccccc1OC
Mol. weight [g/mol]: 412.52

Physical Properties

Property code	Value	Unit	Source
gf	-207.66	kJ/mol	Joback Method
hf	-731.03	kJ/mol	Joback Method
hfus	54.57	kJ/mol	Joback Method
hvap	97.84	kJ/mol	Joback Method
log10ws	-7.53		Crippen Method
logp	5.960		Crippen Method
mcvol	336.340	ml/mol	McGowan Method
pc	1180.09	kPa	Joback Method
rinpol	3474.00		NIST Webbook
rinpol	3474.00		NIST Webbook
tb	1009.72	K	Joback Method
tc	1238.04	K	Joback Method
tf	615.94	K	Joback Method
vc	1.286	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1103.18	J/mol×K	1009.72	Joback Method
cpg	1116.51	J/mol×K	1047.77	Joback Method
cpg	1128.20	J/mol×K	1085.83	Joback Method
cpg	1138.30	J/mol×K	1123.88	Joback Method
cpg	1146.83	J/mol×K	1161.93	Joback Method
cpg	1153.84	J/mol×K	1199.98	Joback Method
cpg	1159.35	J/mol×K	1238.04	Joback Method
dvisc	0.0001892	Pa×s	615.94	Joback Method

dvisc	0.0001097	Pa×s	681.57	Joback Method
dvisc	0.0000700	Pa×s	747.20	Joback Method
dvisc	0.0000480	Pa×s	812.83	Joback Method
dvisc	0.0000348	Pa×s	878.46	Joback Method
dvisc	0.0000264	Pa×s	944.09	Joback Method
dvisc	0.0000208	Pa×s	1009.72	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=U382498&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