Phthalic acid, nonyl 3-phenoxybenzyl ester

Inchi: InChI=1S/C30H34O5/c1-2-3-4-5-6-7-13-21-33-29(31)27-19-11-12-20-28(27)30(32)34-23
InchiKey: LQDCDEUAOYYWBQ-UHFFFAOYSA-N
Formula: C30H34O5
SMILES: CCCCCCCCCOC(=O)c1ccccc1C(=O)OCc1cccc(Oc2ccccc2)c1
Mol. weight [g/mol]: 474.59

Physical Properties

Property code	Value	Unit	Source
gf	-53.15	kJ/mol	Joback Method
hf	-597.70	kJ/mol	Joback Method
hfus	61.56	kJ/mol	Joback Method
hvap	111.25	kJ/mol	Joback Method
log10ws	-9.05		Crippen Method
logp	7.743		Crippen Method
mcvol	383.030	ml/mol	McGowan Method
pc	1067.97	kPa	Joback Method
rinpol	3613.00		NIST Webbook
rinpol	3613.00		NIST Webbook
tb	1150.80	K	Joback Method
tc	1408.97	K	Joback Method
tf	698.71	K	Joback Method
vc	1.458	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1289.86	J/mol×K	1150.80	Joback Method
cpg	1299.70	J/mol×K	1193.83	Joback Method
cpg	1307.63	J/mol×K	1236.86	Joback Method
cpg	1313.74	J/mol×K	1279.88	Joback Method
cpg	1318.12	J/mol×K	1322.91	Joback Method
cpg	1320.85	J/mol×K	1365.94	Joback Method
cpg	1322.04	J/mol×K	1408.97	Joback Method
dvisc	0.0000951	Pa×s	698.71	Joback Method

dvisc	0.0000545	Pa×s	774.06	Joback Method
dvisc	0.0000345	Pa×s	849.41	Joback Method
dvisc	0.0000235	Pa×s	924.75	Joback Method
dvisc	0.0000170	Pa×s	1000.10	Joback Method
dvisc	0.0000129	Pa×s	1075.45	Joback Method
dvisc	0.0000101	Pa×s	1150.80	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=U357040&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