Phthalic acid, heptyl 3-phenoxybenzyl ester

Inchi: InChI=1S/C28H30O5/c1-2-3-4-5-11-19-31-27(29)25-17-9-10-18-26(25)28(30)32-21-22-1
InchiKey: KQFDABCMLHMTMJ-UHFFFAOYSA-N
Formula: C28H30O5
SMILES: CCCCCCCOC(=O)c1ccccc1C(=O)OCc1cccc(Oc2ccccc2)c1
Mol. weight [g/mol]: 446.53

Physical Properties

Property code	Value	Unit	Source
gf	-69.99	kJ/mol	Joback Method
hf	-556.42	kJ/mol	Joback Method
hfus	56.38	kJ/mol	Joback Method
hvap	106.80	kJ/mol	Joback Method
log10ws	-8.21		Crippen Method
logp	6.963		Crippen Method
mcvol	354.850	ml/mol	McGowan Method
pc	1215.74	kPa	Joback Method
rinpol	3404.00		NIST Webbook
rinpol	3404.00		NIST Webbook
tb	1105.04	K	Joback Method
tc	1354.53	K	Joback Method
tf	676.17	K	Joback Method
vc	1.345	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1169.79	J/mol×K	1105.04	Joback Method
cpg	1179.92	J/mol×K	1146.62	Joback Method
cpg	1188.27	J/mol×K	1188.20	Joback Method
cpg	1194.90	J/mol×K	1229.79	Joback Method
cpg	1199.88	J/mol×K	1271.37	Joback Method
cpg	1203.30	J/mol×K	1312.95	Joback Method
cpg	1205.21	J/mol×K	1354.53	Joback Method
dvisc	0.0001220	Pa×s	676.17	Joback Method

dvisc	0.0000712	Pa×s	747.65	Joback Method
dvisc	0.0000457	Pa×s	819.13	Joback Method
dvisc	0.0000315	Pa×s	890.61	Joback Method
dvisc	0.0000229	Pa×s	962.08	Joback Method
dvisc	0.0000174	Pa×s	1033.56	Joback Method
dvisc	0.0000137	Pa×s	1105.04	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357038&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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