Phthalic acid, 3-phenoxybenzyl propyl ester

Inchi: InChI=1S/C24H22O5/c1-2-15-27-23(25)21-13-6-7-14-22(21)24(26)28-17-18-9-8-12-20(1
InchiKey: OHOKXXFKHKPSFR-UHFFFAOYSA-N
Formula: C24H22O5
SMILES: CCCOC(=O)c1ccccc1C(=O)OCc1cccc(Oc2ccccc2)c1
Mol. weight [g/mol]: 390.43

Physical Properties

Property code	Value	Unit	Source
gf	-103.67	kJ/mol	Joback Method
hf	-473.86	kJ/mol	Joback Method
hfus	46.02	kJ/mol	Joback Method
hvap	97.89	kJ/mol	Joback Method
log10ws	-6.54		Crippen Method
logp	5.403		Crippen Method
mcvol	298.490	ml/mol	McGowan Method
pc	1620.68	kPa	Joback Method
rinpol	3040.00		NIST Webbook
tb	1013.52	K	Joback Method
tc	1258.54	K	Joback Method
tf	631.09	K	Joback Method
vc	1.121	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	933.31	J/mol×K	1013.52	Joback Method
cpg	944.01	J/mol×K	1054.36	Joback Method
cpg	953.06	J/mol×K	1095.19	Joback Method
cpg	960.50	J/mol×K	1136.03	Joback Method
cpg	966.39	J/mol×K	1176.87	Joback Method
cpg	970.76	J/mol×K	1217.70	Joback Method
cpg	973.68	J/mol×K	1258.54	Joback Method
dvisc	0.0001945	Pa×s	631.09	Joback Method
dvisc	0.0001182	Pa×s	694.83	Joback Method

dvisc	0.0000781	Pa×s	758.57	Joback Method
dvisc	0.0000550	Pa×s	822.31	Joback Method
dvisc	0.0000408	Pa×s	886.04	Joback Method
dvisc	0.0000315	Pa×s	949.78	Joback Method
dvisc	0.0000251	Pa×s	1013.52	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=U357033&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