Phthalic acid, pent-4-enyl propyl ester

Inchi: InChI=1S/C16H20O4/c1-3-5-8-12-20-16(18)14-10-7-6-9-13(14)15(17)19-11-4-2/h3,6-7,9-
InchiKey: HOYPGSJPTTYNDE-UHFFFAOYSA-N
Formula: C16H20O4
SMILES: C=CCCCOC(=O)c1ccccc1C(=O)OCCC
Mol. weight [g/mol]: 276.33

Physical Properties

Property code	Value	Unit	Source
gf	-193.38	kJ/mol	Joback Method
hf	-512.68	kJ/mol	Joback Method
hfus	35.14	kJ/mol	Joback Method
hvap	71.79	kJ/mol	Joback Method
log10ws	-4.32		Crippen Method
logp	3.376		Crippen Method
mcvol	223.120	ml/mol	McGowan Method
pc	1883.80	kPa	Joback Method
rinpol	1970.00		NIST Webbook
rinpol	1970.00		NIST Webbook
tb	746.40	K	Joback Method
tc	950.98	K	Joback Method
tf	451.58	K	Joback Method
vc	0.853	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	623.45	J/mol×K	746.40	Joback Method
cpg	686.98	J/mol×K	916.89	Joback Method
cpg	676.12	J/mol×K	882.79	Joback Method
cpg	664.35	J/mol×K	848.69	Joback Method
cpg	651.67	J/mol×K	814.59	Joback Method
cpg	638.04	J/mol×K	780.50	Joback Method
cpg	696.94	J/mol×K	950.98	Joback Method
dvisc	0.0000989	Pa×s	746.40	Joback Method

dvisc	0.0001249	Pa×s	697.26	Joback Method
dvisc	0.0001634	Pa×s	648.13	Joback Method
dvisc	0.0002233	Pa×s	598.99	Joback Method
dvisc	0.0003229	Pa×s	549.85	Joback Method
dvisc	0.0005018	Pa×s	500.72	Joback Method
dvisc	0.0008584	Pa×s	451.58	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=U360454&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