Phthalic acid, butyl pent-4-enyl ester

Inchi: InChI=1S/C17H22O4/c1-3-5-9-13-21-17(19)15-11-8-7-10-14(15)16(18)20-12-6-4-2/h3,7-
InchiKey: XGQSDLZUTSZZJA-UHFFFAOYSA-N
Formula: C17H22O4
SMILES: C=CCCCOC(=O)c1ccccc1C(=O)OCCCC
Mol. weight [g/mol]: 290.35

Physical Properties

Property code	Value	Unit	Source
gf	-184.96	kJ/mol	Joback Method
hf	-533.32	kJ/mol	Joback Method
hfus	37.73	kJ/mol	Joback Method
hvap	74.02	kJ/mol	Joback Method
log10ws	-4.74		Crippen Method
logp	3.766		Crippen Method
mcvol	237.210	ml/mol	McGowan Method
pc	1736.11	kPa	Joback Method
rinpol	2062.00		NIST Webbook
rinpol	2062.00		NIST Webbook
tb	769.28	K	Joback Method
tc	972.21	K	Joback Method
tf	462.85	K	Joback Method
vc	0.908	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	678.74	J/mol×K	769.28	Joback Method
cpg	693.64	J/mol×K	803.10	Joback Method
cpg	707.55	J/mol×K	836.92	Joback Method
cpg	720.49	J/mol×K	870.74	Joback Method
cpg	732.48	J/mol×K	904.57	Joback Method
cpg	743.53	J/mol×K	938.39	Joback Method
cpg	753.67	J/mol×K	972.21	Joback Method
dvisc	0.0007930	Pa×s	462.85	Joback Method

dvisc	0.0004572	Pa×s	513.92	Joback Method
dvisc	0.0002912	Pa×s	564.99	Joback Method
dvisc	0.0001999	Pa×s	616.07	Joback Method
dvisc	0.0001453	Pa×s	667.14	Joback Method
dvisc	0.0001106	Pa×s	718.21	Joback Method
dvisc	0.0000872	Pa×s	769.28	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=U360463&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