Phthalic acid, butyl hexyl ester

Other names: Butyl hexyl phthalate
Inchi: InChI=1S/C18H26O4/c1-3-5-7-10-14-22-18(20)16-12-9-8-11-15(16)17(19)21-13-6-4-2/h8
InchiKey: LKVQWLUFJXBHKH-UHFFFAOYSA-N
Formula: C18H26O4
SMILES: CCCCCCOC(=O)c1ccccc1C(=O)OCCCC
Mol. weight [g/mol]: 306.40

Physical Properties

Property code	Value	Unit	Source
gf	-264.38	kJ/mol	Joback Method
hf	-679.39	kJ/mol	Joback Method
hfus	41.60	kJ/mol	Joback Method
hvap	76.91	kJ/mol	Joback Method
log10ws	-5.31		Crippen Method
logp	4.381		Crippen Method
mcvol	255.600	ml/mol	McGowan Method
pc	1552.45	kPa	Joback Method
rinpol	2235.00		NIST Webbook
rinpol	2235.00		NIST Webbook
tb	795.48	K	Joback Method
tc	995.15	K	Joback Method
tf	475.88	K	Joback Method
vc	0.984	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	761.25	J/mol×K	795.48	Joback Method
cpg	776.92	J/mol×K	828.76	Joback Method
cpg	791.55	J/mol×K	862.04	Joback Method
cpg	805.16	J/mol×K	895.32	Joback Method
cpg	817.75	J/mol×K	928.59	Joback Method
cpg	829.35	J/mol×K	961.87	Joback Method
cpg	839.97	J/mol×K	995.15	Joback Method

dvisc	0.0007181	Pa×s	475.88	Joback Method
dvisc	0.0004036	Pa×s	529.15	Joback Method
dvisc	0.0002520	Pa×s	582.41	Joback Method
dvisc	0.0001703	Pa×s	635.68	Joback Method
dvisc	0.0001223	Pa×s	688.95	Joback Method
dvisc	0.0000921	Pa×s	742.21	Joback Method
dvisc	0.0000720	Pa×s	795.48	Joback Method

Sources

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=U308995&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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