

Phthalic acid, butyl trans-hex-3-enyl ester

Inchi:	InChI=1S/C18H24O4/c1-3-5-7-10-14-22-18(20)16-12-9-8-11-15(16)17(19)21-13-6-4-2/h5
InchiKey:	HUXWIYITIHHPIR-FNORWQNLSA-N
Formula:	C18H24O4
SMILES:	CCC=CCCOC(=O)c1ccccc1C(=O)OCCCC
Mol. weight [g/mol]:	304.38

Physical Properties

Property code	Value	Unit	Source
gf	-184.16	kJ/mol	Joback Method
hf	-562.17	kJ/mol	Joback Method
hfus	41.80	kJ/mol	Joback Method
hvap	76.87	kJ/mol	Joback Method
log10ws	-5.16		Crippen Method
logp	4.157		Crippen Method
mcvol	251.300	ml/mol	McGowan Method
pc	1618.07	kPa	Joback Method
rinpol	2155.00		NIST Webbook
tb	799.64	K	Joback Method
tc	1004.52	K	Joback Method
tf	470.80	K	Joback Method
vc	0.964	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	735.73	J/molxK	799.64	Joback Method
cpg	750.91	J/molxK	833.79	Joback Method
cpg	765.08	J/molxK	867.93	Joback Method
cpg	778.26	J/molxK	902.08	Joback Method
cpg	790.48	J/molxK	936.23	Joback Method
cpg	801.78	J/molxK	970.37	Joback Method
cpg	812.18	J/molxK	1004.52	Joback Method
dvisc	0.0006620	Paxs	470.80	Joback Method
dvisc	0.0003640	Paxs	525.61	Joback Method

dvisc	0.0002241	Paxs	580.41	Joback Method
dvisc	0.0001500	Paxs	635.22	Joback Method
dvisc	0.0001070	Paxs	690.03	Joback Method
dvisc	0.0000803	Paxs	744.83	Joback Method
dvisc	0.0000626	Paxs	799.64	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U360482&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
rinpolar:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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