Di(E)-but-2-enyl phthalate

Other names: 1,2-Benzenedicarboxylic acid, di-(E)-but-2-enyl ester
Di(E)-but-2-enyl-1,2-benzenedicarboxylate
Inchi: InChI=1S/C16H18O4/c1-3-5-11-19-15(17)13-9-7-8-10-14(13)16(18)20-12-6-4-2/h3-10H,1
InchiKey: BWGZLWUHRHXHPH-GGWOSOGESA-N
Formula: C16H18O4
SMILES: CC=CCOC(=O)c1ccccc1C(=O)OCC=CC
Mol. weight [g/mol]: 274.31

Physical Properties

Property code	Value	Unit	Source
gf	-120.78	kJ/mol	Joback Method
hf	-403.67	kJ/mol	Joback Method
hfus	36.83	kJ/mol	Joback Method
hvap	72.38	kJ/mol	Joback Method
log10ws	-4.18		Crippen Method
logp	3.152		Crippen Method
mcvol	218.820	ml/mol	McGowan Method
pc	1989.43	kPa	Joback Method
rinpol	2002.00		NIST Webbook
tb	758.04	K	Joback Method
tc	972.83	K	Joback Method
tf	443.18	K	Joback Method
vc	0.832	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	599.23	J/mol×K	758.04	Joback Method
cpg	660.47	J/mol×K	937.03	Joback Method
cpg	649.95	J/mol×K	901.24	Joback Method
cpg	638.61	J/mol×K	865.44	Joback Method
cpg	626.40	J/mol×K	829.64	Joback Method
cpg	613.29	J/mol×K	793.84	Joback Method
cpg	670.20	J/mol×K	972.83	Joback Method

dvisc	0.0000701	Pa×s	758.04	Joback Method
dvisc	0.0000895	Pa×s	705.56	Joback Method
dvisc	0.0001188	Pa×s	653.09	Joback Method
dvisc	0.0001658	Pa×s	600.61	Joback Method
dvisc	0.0002465	Pa×s	548.13	Joback Method
dvisc	0.0003985	Pa×s	495.66	Joback Method
dvisc	0.0007221	Pa×s	443.18	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U373500&Units=SI
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

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