Terephthalic acid, but-3-enyl ethyl ester

Inchi: InChI=1S/C14H16O4/c1-3-5-10-18-14(16)12-8-6-11(7-9-12)13(15)17-4-2/h3,6-9H,1,4-5,1
InchiKey: KJIHSRJQMXXEGN-UHFFFAOYSA-N
Formula: C14H16O4
SMILES: C=CCCOC(=O)c1ccc(C(=O)OCC)cc1
Mol. weight [g/mol]: 248.27

Physical Properties

Property code	Value	Unit	Source
gf	-210.22	kJ/mol	Joback Method
hf	-471.40	kJ/mol	Joback Method
hfus	29.96	kJ/mol	Joback Method
hvap	67.34	kJ/mol	Joback Method
log10ws	-3.48		Crippen Method
logp	2.596		Crippen Method
mcvol	194.940	ml/mol	McGowan Method
pc	2241.88	kPa	Joback Method
rinpol	1889.00		NIST Webbook
tb	700.64	K	Joback Method
tc	910.00	K	Joback Method
tf	429.04	K	Joback Method
vc	0.741	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	516.26	J/mol×K	700.64	Joback Method
cpg	576.47	J/mol×K	875.11	Joback Method
cpg	566.16	J/mol×K	840.21	Joback Method
cpg	554.99	J/mol×K	805.32	Joback Method
cpg	542.96	J/mol×K	770.43	Joback Method
cpg	530.06	J/mol×K	735.53	Joback Method
cpg	585.94	J/mol×K	910.00	Joback Method
dvisc	0.0001255	Pa×s	700.64	Joback Method
dvisc	0.0001572	Pa×s	655.37	Joback Method

dvisc	0.0002035	Pa×s	610.11	Joback Method
dvisc	0.0002747	Pa×s	564.84	Joback Method
dvisc	0.0003906	Pa×s	519.57	Joback Method
dvisc	0.0005940	Pa×s	474.31	Joback Method
dvisc	0.0009868	Pa×s	429.04	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U356333&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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