Terephthalic acid, but-3-enyl propyl ester

Inchi: InChI=1S/C15H18O4/c1-3-5-11-19-15(17)13-8-6-12(7-9-13)14(16)18-10-4-2/h3,6-9H,1,4
InchiKey: CKYKRJSNKQFRSU-UHFFFAOYSA-N
Formula: C15H18O4
SMILES: C=CCCOC(=O)c1ccc(C(=O)OCCC)cc1
Mol. weight [g/mol]: 262.30

Physical Properties

Property code	Value	Unit	Source
gf	-201.80	kJ/mol	Joback Method
hf	-492.04	kJ/mol	Joback Method
hfus	32.55	kJ/mol	Joback Method
hvap	69.56	kJ/mol	Joback Method
log10ws	-3.90		Crippen Method
logp	2.986		Crippen Method
mcvol	209.030	ml/mol	McGowan Method
pc	2051.17	kPa	Joback Method
rinpol	1999.00		NIST Webbook
rinpol	1999.00		NIST Webbook
tb	723.52	K	Joback Method
tc	930.26	K	Joback Method
tf	440.31	K	Joback Method
vc	0.796	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	569.26	J/mol×K	723.52	Joback Method
cpg	631.28	J/mol×K	895.80	Joback Method
cpg	620.66	J/mol×K	861.35	Joback Method
cpg	609.17	J/mol×K	826.89	Joback Method
cpg	596.78	J/mol×K	792.43	Joback Method
cpg	583.49	J/mol×K	757.98	Joback Method
cpg	641.02	J/mol×K	930.26	Joback Method
dvisc	0.0001117	Pa×s	723.52	Joback Method

dvisc	0.0001404	Pa×s	676.32	Joback Method
dvisc	0.0001828	Pa×s	629.12	Joback Method
dvisc	0.0002483	Pa×s	581.91	Joback Method
dvisc	0.0003561	Pa×s	534.71	Joback Method
dvisc	0.0005476	Pa×s	487.51	Joback Method
dvisc	0.0009235	Pa×s	440.31	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=U356334&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