Terephthalic acid, but-3-enyl hexyl ester

Inchi: InChI=1S/C18H24O4/c1-3-5-7-8-14-22-18(20)16-11-9-15(10-12-16)17(19)21-13-6-4-2/h4
InchiKey: GOCUZZWHKYALTN-UHFFFAOYSA-N
Formula: C18H24O4
SMILES: C=CCCOC(=O)c1ccc(C(=O)OCCCCCC)cc1
Mol. weight [g/mol]: 304.38

Physical Properties

Property code	Value	Unit	Source
gf	-176.54	kJ/mol	Joback Method
hf	-553.96	kJ/mol	Joback Method
hfus	40.32	kJ/mol	Joback Method
hvap	76.24	kJ/mol	Joback Method
log10ws	-5.16		Crippen Method
logp	4.157		Crippen Method
mcvol	251.300	ml/mol	McGowan Method
pc	1605.13	kPa	Joback Method
rinpol	2328.00		NIST Webbook
rinpol	2328.00		NIST Webbook
tb	792.16	K	Joback Method
tc	993.99	K	Joback Method
tf	474.12	K	Joback Method
vc	0.965	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	735.06	J/mol×K	792.16	Joback Method
cpg	800.91	J/mol×K	960.35	Joback Method
cpg	789.70	J/mol×K	926.71	Joback Method
cpg	777.53	J/mol×K	893.07	Joback Method
cpg	764.38	J/mol×K	859.44	Joback Method
cpg	750.23	J/mol×K	825.80	Joback Method
cpg	811.19	J/mol×K	993.99	Joback Method
dvisc	0.0000767	Pa×s	792.16	Joback Method

dvisc	0.0000975	Pa×s	739.15	Joback Method
dvisc	0.0001288	Pa×s	686.15	Joback Method
dvisc	0.0001781	Pa×s	633.14	Joback Method
dvisc	0.0002614	Pa×s	580.13	Joback Method
dvisc	0.0004144	Pa×s	527.13	Joback Method
dvisc	0.0007284	Pa×s	474.12	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=U356336&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