Terephthalic acid, but-3-enyl isohexyl ester

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

Physical Properties

Property code	Value	Unit	Source
gf	-178.98	kJ/mol	Joback Method
hf	-559.24	kJ/mol	Joback Method
hfus	36.80	kJ/mol	Joback Method
hvap	75.85	kJ/mol	Joback Method
log10ws	-4.92		Crippen Method
logp	4.013		Crippen Method
mcvol	251.300	ml/mol	McGowan Method
pc	1615.47	kPa	Joback Method
rinpol	2287.00		NIST Webbook
rinpol	2287.00		NIST Webbook
tb	791.72	K	Joback Method
tc	996.07	K	Joback Method
tf	459.12	K	Joback Method
vc	0.959	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	735.60	J/mol×K	791.72	Joback Method
cpg	750.96	J/mol×K	825.78	Joback Method
cpg	765.27	J/mol×K	859.84	Joback Method
cpg	778.54	J/mol×K	893.90	Joback Method
cpg	790.79	J/mol×K	927.95	Joback Method
cpg	802.05	J/mol×K	962.01	Joback Method
cpg	812.34	J/mol×K	996.07	Joback Method
dvisc	0.0008308	Pa×s	459.12	Joback Method

dvisc	0.0004413	Pa×s	514.55	Joback Method
dvisc	0.0002651	Pa×s	569.99	Joback Method
dvisc	0.0001743	Pa×s	625.42	Joback Method
dvisc	0.0001227	Pa×s	680.85	Joback Method
dvisc	0.0000910	Pa×s	736.29	Joback Method
dvisc	0.0000705	Pa×s	791.72	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=U356335&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

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