Terephthalic acid, but-3-enyl hexadecyl ester

Inchi: InChI=1S/C28H44O4/c1-3-5-7-8-9-10-11-12-13-14-15-16-17-18-24-32-28(30)26-21-19-2
InchiKey: XCVVRVDBEWZCDT-UHFFFAOYSA-N
Formula: C28H44O4
SMILES: C=CCCOC(=O)c1ccc(C(=O)OCCCCCCCCCCCCCCCC)cc1
Mol. weight [g/mol]: 444.65

Physical Properties

Property code	Value	Unit	Source
gf	-92.34	kJ/mol	Joback Method
hf	-760.36	kJ/mol	Joback Method
hfus	66.22	kJ/mol	Joback Method
hvap	98.50	kJ/mol	Joback Method
log10ws	-9.34		Crippen Method
logp	8.058		Crippen Method
mcvol	392.200	ml/mol	McGowan Method
pc	837.24	kPa	Joback Method
rinpol	3397.00		NIST Webbook
tb	1020.96	K	Joback Method
tc	1253.49	K	Joback Method
tf	586.82	K	Joback Method
vc	1.524	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1339.18	J/mol×K	1020.96	Joback Method
cpg	1412.36	J/mol×K	1214.74	Joback Method
cpg	1400.74	J/mol×K	1175.98	Joback Method
cpg	1387.69	J/mol×K	1137.23	Joback Method
cpg	1373.13	J/mol×K	1098.47	Joback Method
cpg	1356.99	J/mol×K	1059.72	Joback Method
cpg	1422.61	J/mol×K	1253.49	Joback Method
dvisc	0.0000181	Pa×s	1020.96	Joback Method
dvisc	0.0000237	Pa×s	948.60	Joback Method

dvisc	0.0000325	Pa×s	876.25	Joback Method
dvisc	0.0000470	Pa×s	803.89	Joback Method
dvisc	0.0000732	Pa×s	731.53	Joback Method
dvisc	0.0001257	Pa×s	659.18	Joback Method
dvisc	0.0002465	Pa×s	586.82	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U356346&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