Terephthalic acid, but-3-enyl tridecyl ester

Inchi: InChI=1S/C25H38O4/c1-3-5-7-8-9-10-11-12-13-14-15-21-29-25(27)23-18-16-22(17-19-2
InchiKey: YCEVAJOGSYXNPQ-UHFFFAOYSA-N
Formula: C25H38O4
SMILES: C=CCCOC(=O)c1ccc(C(=O)OCCCCCCCCCCCCC)cc1
Mol. weight [g/mol]: 402.57

Physical Properties

Property code	Value	Unit	Source
gf	-117.60	kJ/mol	Joback Method
hf	-698.44	kJ/mol	Joback Method
hfus	58.45	kJ/mol	Joback Method
hvap	91.82	kJ/mol	Joback Method
log10ws	-8.09		Crippen Method
logp	6.887		Crippen Method
mcvol	349.930	ml/mol	McGowan Method
pc	996.39	kPa	Joback Method
rinpol	3076.00		NIST Webbook
rinpol	3076.00		NIST Webbook
tb	952.32	K	Joback Method
tc	1166.01	K	Joback Method
tf	553.01	K	Joback Method
vc	1.357	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1151.84	J/mol×K	952.32	Joback Method
cpg	1168.68	J/mol×K	987.94	Joback Method
cpg	1184.14	J/mol×K	1023.55	Joback Method
cpg	1198.27	J/mol×K	1059.17	Joback Method
cpg	1211.14	J/mol×K	1094.78	Joback Method
cpg	1222.77	J/mol×K	1130.40	Joback Method
cpg	1233.23	J/mol×K	1166.01	Joback Method
dvisc	0.0003540	Pa×s	553.01	Joback Method

dvisc	0.0001858	Pa×s	619.56	Joback Method
dvisc	0.0001105	Pa×s	686.11	Joback Method
dvisc	0.0000721	Pa×s	752.66	Joback Method
dvisc	0.0000504	Pa×s	819.22	Joback Method
dvisc	0.0000372	Pa×s	885.77	Joback Method
dvisc	0.0000286	Pa×s	952.32	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U356343&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