

Terephthalic acid, but-3-enyl decyl ester

Inchi: InChI=1S/C22H32O4/c1-3-5-7-8-9-10-11-12-18-26-22(24)20-15-13-19(14-16-20)21(23)2
InchiKey: RXYZCQFRFQXQSR-UHFFFAOYSA-N
Formula: C22H32O4
SMILES: C=CCCCOC(=O)c1ccc(C(=O)OCCCCCCCCCCC)cc1
Mol. weight [g/mol]: 360.49

Physical Properties

Property code	Value	Unit	Source
gf	-142.86	kJ/mol	Joback Method
hf	-636.52	kJ/mol	Joback Method
hfus	50.68	kJ/mol	Joback Method
hvap	85.15	kJ/mol	Joback Method
log10ws	-6.83		Crippen Method
logp	5.717		Crippen Method
mcvol	307.660	ml/mol	McGowan Method
pc	1205.63	kPa	Joback Method
rinpol	2755.00		NIST Webbook
tb	883.68	K	Joback Method
tc	1087.55	K	Joback Method
tf	519.20	K	Joback Method
vc	1.188	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	969.05	J/molxK	883.68	Joback Method
cpg	985.14	J/molxK	917.66	Joback Method
cpg	1000.05	J/molxK	951.64	Joback Method
cpg	1013.81	J/molxK	985.61	Joback Method
cpg	1026.45	J/molxK	1019.59	Joback Method
cpg	1038.00	J/molxK	1053.57	Joback Method
cpg	1048.51	J/molxK	1087.55	Joback Method
dvisc	0.0004940	Paxs	519.20	Joback Method
dvisc	0.0002678	Paxs	579.95	Joback Method

dvisc	0.0001630	Paxs	640.69	Joback Method
dvisc	0.0001082	Paxs	701.44	Joback Method
dvisc	0.0000766	Paxs	762.19	Joback Method
dvisc	0.0000571	Paxs	822.93	Joback Method
dvisc	0.0000443	Paxs	883.68	Joback Method

Sources

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=U356340&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

Latest version available from:

<https://www.chemeo.com/cid/34-862-7/Terephthalic-acid-but-3-enyl-decyl-ester.pdf>

Generated by Cheméo on 2024-04-24 16:14:25.562574963 +0000 UTC m=+16264514.483152318.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.