

Terephthalic acid, but-2-enyl octyl ester

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C20H28O4/c1-3-5-7-8-9-10-16-24-20(22)18-13-11-17(12-14-18)19(21)23-15-6

PPVUHSQYAWEMJE-GQCTYLIASA-N

C20H28O4

CC=CCOC(=O)c1ccc(C(=O)OCCCCCCCC)cc1

332.43

Physical Properties

Property code	Value	Unit	Source
gf	-167.32	kJ/mol	Joback Method
hf	-603.45	kJ/mol	Joback Method
hfus	46.98	kJ/mol	Joback Method
hvap	81.32	kJ/mol	Joback Method
log10ws	-6.00		Crippen Method
logp	4.937		Crippen Method
mcvol	279.480	ml/mol	McGowan Method
pc	1394.37	kPa	Joback Method
rinpol	2581.00		NIST Webbook
tb	845.40	K	Joback Method
tc	1049.53	K	Joback Method
tf	493.34	K	Joback Method
vc	1.075	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	851.27	J/mol×K	845.40	Joback Method
cpg	866.94	J/mol×K	879.42	Joback Method
cpg	881.53	J/mol×K	913.44	Joback Method
cpg	895.08	J/mol×K	947.46	Joback Method
cpg	907.62	J/mol×K	981.48	Joback Method
cpg	919.19	J/mol×K	1015.50	Joback Method
cpg	929.83	J/mol×K	1049.53	Joback Method
dvisc	0.0005474	Pa×s	493.34	Joback Method
dvisc	0.0002938	Pa×s	552.02	Joback Method

dvisc	0.0001777	Pa×s	610.69	Joback Method
dvisc	0.0001174	Pa×s	669.37	Joback Method
dvisc	0.0000829	Pa×s	728.05	Joback Method
dvisc	0.0000617	Pa×s	786.72	Joback Method
dvisc	0.0000478	Pa×s	845.40	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=U356316&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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