

Terephthalic acid, but-3-enyl heptyl ester

Inchi:	InChI=1S/C19H26O4/c1-3-5-7-8-9-15-23-19(21)17-12-10-16(11-13-17)18(20)22-14-6-4-2
InchiKey:	PFVSIQAQAWKCZJK-UHFFFAOYSA-N
Formula:	C19H26O4
SMILES:	<chem>C=CCCOC(=O)c1ccc(C(=O)OCCCCCCC)cc1</chem>
Mol. weight [g/mol]:	318.41

Physical Properties

Property code	Value	Unit	Source
gf	-168.12	kJ/mol	Joback Method
hf	-574.60	kJ/mol	Joback Method
hfus	42.91	kJ/mol	Joback Method
hvap	78.47	kJ/mol	Joback Method
log10ws	-5.58		Crippen Method
logp	4.547		Crippen Method
mcvol	265.390	ml/mol	McGowan Method
pc	1488.44	kPa	Joback Method
rinsol	2435.00		NIST Webbook
tb	815.04	K	Joback Method
tc	1016.36	K	Joback Method
tf	485.39	K	Joback Method
vc	1.020	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	792.31	J/molxK	815.04	Joback Method
cpg	807.73	J/molxK	848.59	Joback Method
cpg	822.10	J/molxK	882.15	Joback Method
cpg	835.43	J/molxK	915.70	Joback Method
cpg	847.75	J/molxK	949.25	Joback Method
cpg	859.08	J/molxK	982.80	Joback Method
cpg	869.46	J/molxK	1016.36	Joback Method
dvisc	0.0006656	Paxs	485.39	Joback Method
dvisc	0.0003739	Paxs	540.33	Joback Method

dvisc	0.0002336	Paxs	595.27	Joback Method
dvisc	0.0001580	Paxs	650.21	Joback Method
dvisc	0.0001136	Paxs	705.16	Joback Method
dvisc	0.0000857	Paxs	760.10	Joback Method
dvisc	0.0000671	Paxs	815.04	Joback Method

Sources

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=U356337&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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