

Terephthalic acid, di(but-3-enyl) ester

Inchi:	InChI=1S/C16H18O4/c1-3-5-11-19-15(17)13-7-9-14(10-8-13)16(18)20-12-6-4-2/h3-4,7-1
InchiKey:	TVHCSJSGHDPGEW-UHFFFAOYSA-N
Formula:	C16H18O4
SMILES:	C=CCCOC(=O)c1ccc(C(=O)OCCC=C)cc1
Mol. weight [g/mol]:	274.31

Physical Properties

Property code	Value	Unit	Source
gf	-105.54	kJ/mol	Joback Method
hf	-387.25	kJ/mol	Joback Method
hfus	33.86	kJ/mol	Joback Method
hvap	71.12	kJ/mol	Joback Method
log10ws	-4.18		Crippen Method
logp	3.152		Crippen Method
mvol	218.820	ml/mol	McGowan Method
pc	1954.41	kPa	Joback Method
rinpol	2108.00		NIST Webbook
rinpol	2108.00		NIST Webbook
tb	743.08	K	Joback Method
tc	950.66	K	Joback Method
tf	449.82	K	Joback Method
vc	0.834	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	598.61	J/molxK	743.08	Joback Method
cpg	612.64	J/molxK	777.68	Joback Method
cpg	625.73	J/molxK	812.27	Joback Method
cpg	637.90	J/molxK	846.87	Joback Method
cpg	649.17	J/molxK	881.46	Joback Method
cpg	659.55	J/molxK	916.06	Joback Method
cpg	669.08	J/molxK	950.66	Joback Method
dvisc	0.0008637	Paxs	449.82	Joback Method

dvisc	0.0005114	Paxs	498.70	Joback Method
dvisc	0.0003325	Paxs	547.57	Joback Method
dvisc	0.0002320	Paxs	596.45	Joback Method
dvisc	0.0001709	Paxs	645.33	Joback Method
dvisc	0.0001315	Paxs	694.20	Joback Method
dvisc	0.0001047	Paxs	743.08	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U356368&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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