Terephthalic acid, 3-methoxyphenyl propyl ester

Inchi: InChI=1S/C18H18O5/c1-3-11-22-17(19)13-7-9-14(10-8-13)18(20)23-16-6-4-5-15(12-16)2

InchiKey: XOTRMVYOYOAPRM-UHFFFAOYSA-N

Formula: C18H18O5

SMILES: CCCOC(=O)c1ccc(C(=O)Oc2cccc(OC)c2)cc1

Mol. weight [g/mol]: 314.33

Physical Properties

Property code	Value	Unit	Source
gf	-266.60	kJ/mol	Joback Method
hf	-586.55	kJ/mol	Joback Method
hfus	36.44	kJ/mol	Joback Method
hvap	82.26	kJ/mol	Joback Method
log10ws	-4.76		Crippen Method
logp	3.481		Crippen Method
mcvol	237.710	ml/mol	McGowan Method
pc	1994.77	kPa	Joback Method
rinpol	2654.00		NIST Webbook
rinpol	2654.00		NIST Webbook
tb	849.56	K	Joback Method
tc	1077.01	K	Joback Method
tf	537.05	K	Joback Method
vc	0.893	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	693.56	J/mol×K	849.56	Joback Method
cpg	706.79	J/mol×K	887.47	Joback Method
cpg	718.71	J/mol×K	925.38	Joback Method
cpg	729.32	J/mol×K	963.28	Joback Method
cpg	738.65	J/mol×K	1001.19	Joback Method
cpg	746.68	J/mol×K	1039.10	Joback Method
cpg	753.43	J/mol×K	1077.01	Joback Method
dvisc	0.0003908	Pa×s	537.05	Joback Method

dvisc	0.0002454	Pa×s	589.13	Joback Method
dvisc	0.0001661	Pa×s	641.22	Joback Method
dvisc	0.0001193	Pa×s	693.31	Joback Method
dvisc	0.0000897	Pa×s	745.39	Joback Method
dvisc	0.0000700	Pa×s	797.47	Joback Method
dvisc	0.0000563	Pa×s	849.56	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415818&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

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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