Terephthalic acid, ethyl 2-phenoxyethyl ester

Inchi: InChI=1S/C18H18O5/c1-2-21-17(19)14-8-10-15(11-9-14)18(20)23-13-12-22-16-6-4-3-5-7
InchiKey: CIRPOMNPTNEWJZ-UHFFFAOYSA-N
Formula: C18H18O5
SMILES: CCOC(=O)c1ccc(C(=O)OCCOc2ccccc2)cc1
Mol. weight [g/mol]: 314.33

Physical Properties

Property code	Value	Unit	Source
gf	-256.97	kJ/mol	Joback Method
hf	-575.08	kJ/mol	Joback Method
hfus	36.83	kJ/mol	Joback Method
hvap	81.60	kJ/mol	Joback Method
log10ws	-4.14		Crippen Method
logp	3.099		Crippen Method
mcvol	237.710	ml/mol	McGowan Method
pc	2021.76	kPa	Joback Method
rinpol	2622.00		NIST Webbook
rinpol	2622.00		NIST Webbook
tb	844.58	K	Joback Method
tc	1071.29	K	Joback Method
tf	524.53	K	Joback Method
vc	0.893	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	694.84	J/mol×K	844.58	Joback Method
cpg	748.63	J/mol×K	1033.50	Joback Method
cpg	740.42	J/mol×K	995.72	Joback Method
cpg	730.95	J/mol×K	957.93	Joback Method
cpg	720.21	J/mol×K	920.15	Joback Method
cpg	708.18	J/mol×K	882.36	Joback Method
cpg	755.59	J/mol×K	1071.29	Joback Method
dvisc	0.0000556	Pa×s	844.58	Joback Method

dvisc	0.0000699	Pa×s	791.24	Joback Method
dvisc	0.0000910	Pa×s	737.90	Joback Method
dvisc	0.0001233	Pa×s	684.55	Joback Method
dvisc	0.0001759	Pa×s	631.21	Joback Method
dvisc	0.0002680	Pa×s	577.87	Joback Method
dvisc	0.0004449	Pa×s	524.53	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U416040&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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