Phthalic acid, ethyl 5-ethyl-1,3-dioxan-5-yl ester

Inchi: InChI=1S/C17H22O6/c1-3-17(9-20-12-21-10-17)11-23-16(19)14-8-6-5-7-13(14)15(18)22

InchiKey: JTPBZNSGYBLDSK-UHFFFAOYSA-N

Formula: C17H22O6

SMILES: CCOC(=O)c1ccccc1C(=O)OCC1(CC)COCOC1

Mol. weight [g/mol]: 322.35

Physical Properties

Property code	Value	Unit	Source
gf	-426.08	kJ/mol	Joback Method
hf	-853.19	kJ/mol	Joback Method
hfus	40.51	kJ/mol	Joback Method
hvap	82.98	kJ/mol	Joback Method
log10ws	-3.21		Crippen Method
logp	2.421		Crippen Method
mcvol	242.390	ml/mol	McGowan Method
pc	2047.46	kPa	Joback Method
rinpol	2435.00		NIST Webbook
rinpol	2435.00		NIST Webbook
tb	846.29	K	Joback Method
tc	1075.41	K	Joback Method
tf	549.03	K	Joback Method
vc	0.900	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	757.69	J/mol×K	846.29	Joback Method
cpg	774.48	J/mol×K	884.48	Joback Method
cpg	790.54	J/mol×K	922.66	Joback Method
cpg	805.98	J/mol×K	960.85	Joback Method
cpg	820.92	J/mol×K	999.04	Joback Method
cpg	835.49	J/mol×K	1037.22	Joback Method
cpg	849.79	J/mol×K	1075.41	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=U415477&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
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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