Terephthalic acid, di((5-ethyl-1,3-dioxan-5-yl)methyl) ester

Inchi: InChI=1S/C22H30O8/c1-3-21(9-25-15-26-10-21)13-29-19(23)17-5-7-18(8-6-17)20(24)30
InchiKey: PXJAMMPILFAJIR-UHFFFAOYSA-N
Formula: C22H30O8
SMILES: CCC1(COC(=O)c2ccc(C(=O)OCC3(CC)COCOC3)cc2)COCOC1
Mol. weight [g/mol]: 422.47

Physical Properties

Property code	Value	Unit	Source
gf	-537.26	kJ/mol	Joback Method
hf	-1150.83	kJ/mol	Joback Method
hfus	54.95	kJ/mol	Joback Method
hvap	102.41	kJ/mol	Joback Method
log10ws	-3.63		Crippen Method
logp	2.802		Crippen Method
mcvol	313.720	ml/mol	McGowan Method
pc	1655.15	kPa	Joback Method
rinpol	3664.00		NIST Webbook
rinpol	3664.00		NIST Webbook
tb	1034.38	K	Joback Method
tc	1282.10	K	Joback Method
tf	689.80	K	Joback Method
vc	1.153	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1131.50	J/mol×K	1034.38	Joback Method
cpg	1156.91	J/mol×K	1075.67	Joback Method
cpg	1183.09	J/mol×K	1116.95	Joback Method
cpg	1210.32	J/mol×K	1158.24	Joback Method
cpg	1238.90	J/mol×K	1199.53	Joback Method
cpg	1269.13	J/mol×K	1240.81	Joback Method
cpg	1301.31	J/mol×K	1282.10	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=U383010&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