6H,12H,18H-Tribenzo[b,f,j][1,5,9]trioxacyclododec-6,12,18-tri(oxo)-

Inchi: InChI=1S/C21H12O6/c22-19-13-7-1-4-10-16(13)25-20(23)15-9-3-6-12-18(15)27-21(24)1
InchiKey: KYLIMUJRJDIPPF-UHFFFAOYSA-N
Formula: C21H12O6
SMILES: O=C1Oc2ccccc2C(=O)Oc2ccccc2C(=O)Oc2ccccc21
Mol. weight [g/mol]: 360.32

Physical Properties

Property code	Value	Unit	Source
gf	-159.69	kJ/mol	Joback Method
hf	-536.03	kJ/mol	Joback Method
hfus	44.33	kJ/mol	Joback Method
hvap	98.16	kJ/mol	Joback Method
log10ws	-5.98		Crippen Method
logp	3.658		Crippen Method
mcvol	246.930	ml/mol	McGowan Method
pc	2576.72	kPa	Joback Method
rinpol	3228.00		NIST Webbook
rinpol	3228.00		NIST Webbook
tb	1083.39	K	Joback Method
tc	1383.53	K	Joback Method
tf	739.24	K	Joback Method
vc	0.905	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	785.49	J/mol×K	1083.39	Joback Method
cpg	788.98	J/mol×K	1133.41	Joback Method
cpg	789.12	J/mol×K	1183.44	Joback Method
cpg	785.85	J/mol×K	1233.46	Joback Method
cpg	779.10	J/mol×K	1283.49	Joback Method
cpg	768.80	J/mol×K	1333.51	Joback Method
cpg	754.90	J/mol×K	1383.53	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U375152&Units=SI

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