Howflex gbp

Other names: 3,4,6,7-tetrahydro-2,5,8-benzotrioxacycloundecin-1,9-dione
Inchi: InChI=1S/C12H12O5/c13-11-9-3-1-2-4-10(9)12(14)17-8-6-15-5-7-16-11/h1-4H,5-8H2
InchiKey: LZEGUDFMCKJMPX-UHFFFAOYSA-N
Formula: C12H12O5
SMILES: O=C1OCCOCCOC(=O)c2ccccc21
Mol. weight [g/mol]: 236.22
CAS: 13988-26-6

Physical Properties

Property code	Value	Unit	Source
gf	-354.74	kJ/mol	Joback Method
hf	-681.17	kJ/mol	Joback Method
hfus	27.91	kJ/mol	Joback Method
hvap	68.52	kJ/mol	Joback Method
log10ws	-1.78		Crippen Method
logp	1.030		Crippen Method
mcvol	166.070	ml/mol	McGowan Method
pc	3468.36	kPa	Joback Method
rinpol	1947.00		NIST Webbook
rinpol	1947.00		NIST Webbook
rinpol	1947.00		NIST Webbook
tb	759.14	K	Joback Method
tc	1040.15	K	Joback Method
tf	481.15	K	Joback Method
vc	0.587	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	492.00	J/mol×K	759.14	Joback Method
cpg	509.28	J/mol×K	805.97	Joback Method
cpg	524.47	J/mol×K	852.81	Joback Method
cpg	537.46	J/mol×K	899.64	Joback Method
cpg	548.16	J/mol×K	946.48	Joback Method

cpg	556.45	J/mol×K	993.31	Joback Method
cpg	562.23	J/mol×K	1040.15	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C13988266&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
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