Hexahydro-3-butylphthalide

Inchi: InChI=1S/C12H20O2/c1-2-3-8-11-9-6-4-5-7-10(9)12(13)14-11/h9-11H,2-8H2,1H3
InchiKey: TZRMFZSOOVBPPN-UHFFFAOYSA-N
Formula: C12H20O2
SMILES: CCCCC1OC(=O)C2CCCCC12
Mol. weight [g/mol]: 196.29
CAS: 3553-34-2

Physical Properties

Property code	Value	Unit	Source
gf	-81.06	kJ/mol	Joback Method
hf	-453.93	kJ/mol	Joback Method
hfus	25.37	kJ/mol	Joback Method
hvap	51.10	kJ/mol	Joback Method
log10ws	-3.13		Crippen Method
logp	2.908		Crippen Method
mcvol	165.660	ml/mol	McGowan Method
pc	2398.22	kPa	Joback Method
rinpol	1645.80		NIST Webbook
tb	590.35	K	Joback Method
tc	810.19	K	Joback Method
tf	340.87	K	Joback Method
vc	0.625	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	459.11	J/mol×K	590.35	Joback Method
cpg	479.95	J/mol×K	626.99	Joback Method
cpg	499.59	J/mol×K	663.63	Joback Method
cpg	518.06	J/mol×K	700.27	Joback Method
cpg	535.39	J/mol×K	736.91	Joback Method
cpg	551.59	J/mol×K	773.55	Joback Method
cpg	566.71	J/mol×K	810.19	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3553342&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
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