3-(1'-methylbutylidene)-4,5-dihydrophthalide

Inchi: InChI=1S/C13H18O/c1-3-6-10(2)13-12-8-5-4-7-11(12)9-14-13/h4,7H,3,5-6,8-9H2,1-2H3/
InchiKey: JKOMDTBYVZIMAG-RAXLEYEMSA-N
Formula: C13H18O
SMILES: CCCC(C)=C1OCC2=C1CCC=C2
Mol. weight [g/mol]: 190.28

Physical Properties

Property code	Value	Unit	Source
gf	150.65	kJ/mol	Joback Method
hf	-116.99	kJ/mol	Joback Method
hfus	25.91	kJ/mol	Joback Method
hvap	52.78	kJ/mol	Joback Method
log10ws	-4.20		Crippen Method
logp	3.737		Crippen Method
mcvol	165.280	ml/mol	McGowan Method
pc	2505.01	kPa	Joback Method
rinpol	1702.00		NIST Webbook
tb	574.22	K	Joback Method
tc	793.83	K	Joback Method
tf	319.60	K	Joback Method
vc	0.632	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	410.98	J/mol×K	574.22	Joback Method
cpg	428.21	J/mol×K	610.82	Joback Method
cpg	444.33	J/mol×K	647.42	Joback Method
cpg	459.42	J/mol×K	684.03	Joback Method
cpg	473.55	J/mol×K	720.63	Joback Method
cpg	486.80	J/mol×K	757.23	Joback Method
cpg	499.26	J/mol×K	793.83	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=R219319&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