3n-valeryl-4,5-dihydrophthalide

Inchi: InChI=1S/C13H18O/c1-2-3-4-9-13-12-8-6-5-7-11(12)10-14-13/h5,7,9H,2-4,6,8,10H2,1H3
InchiKey: ZLAFQLXVGWHNRT-LCYFTJDESA-N
Formula: C13H18O
SMILES: CCCCC=C1OCC2=C1CCC=C2
Mol. weight [g/mol]: 190.28

Physical Properties

Property code	Value	Unit	Source
gf	159.20	kJ/mol	Joback Method
hf	-107.20	kJ/mol	Joback Method
hfus	27.22	kJ/mol	Joback Method
hvap	52.70	kJ/mol	Joback Method
log10ws	-4.20		Crippen Method
logp	3.737		Crippen Method
mcvol	165.280	ml/mol	McGowan Method
pc	2492.52	kPa	Joback Method
rinpol	1767.00		NIST Webbook
rinpol	1767.00		NIST Webbook
tb	574.34	K	Joback Method
tc	790.03	K	Joback Method
tf	333.56	K	Joback Method
vc	0.631	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	411.20	J/mol×K	574.34	Joback Method
cpg	428.16	J/mol×K	610.29	Joback Method
cpg	444.04	J/mol×K	646.24	Joback Method
cpg	458.93	J/mol×K	682.18	Joback Method
cpg	472.88	J/mol×K	718.13	Joback Method
cpg	485.98	J/mol×K	754.08	Joback Method
cpg	498.30	J/mol×K	790.03	Joback Method
dvisc	0.0021356	Pa×s	333.56	Joback Method

dvisc	0.0013346	Pa×s	373.69	Joback Method
dvisc	0.0009137	Pa×s	413.82	Joback Method
dvisc	0.0006689	Pa×s	453.95	Joback Method
dvisc	0.0005151	Pa×s	494.08	Joback Method
dvisc	0.0004125	Pa×s	534.21	Joback Method
dvisc	0.0003408	Pa×s	574.34	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R219324&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
dvisc:	Dynamic viscosity
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