Butylidene dihydrophthalide

Inchi: InChI=1S/C12H14O2/c1-2-3-8-11-9-6-4-5-7-10(9)12(13)14-11/h4-5,7-9H,2-3,6H2,1H3/b1
InchiKey: HYBKZIMAEUOFDE-FLIBITNWSA-N
Formula: C12H14O2
SMILES: CCCC=C1OC(=O)C2=CC=CCC12
Mol. weight [g/mol]: 190.24

Physical Properties

Property code	Value	Unit	Source
gf	30.11	kJ/mol	Joback Method
hf	-233.13	kJ/mol	Joback Method
hfus	25.60	kJ/mol	Joback Method
hvap	53.75	kJ/mol	Joback Method
log10ws	-3.31		Crippen Method
logp	2.730		Crippen Method
mcvol	152.760	ml/mol	McGowan Method
pc	2799.47	kPa	Joback Method
rinpol	1734.00		NIST Webbook
tb	609.63	K	Joback Method
tc	841.65	K	Joback Method
tf	373.75	K	Joback Method
vc	0.582	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	393.96	J/mol×K	609.63	Joback Method
cpg	410.19	J/mol×K	648.30	Joback Method
cpg	425.37	J/mol×K	686.97	Joback Method
cpg	439.56	J/mol×K	725.64	Joback Method
cpg	452.80	J/mol×K	764.31	Joback Method
cpg	465.13	J/mol×K	802.98	Joback Method
cpg	476.61	J/mol×K	841.65	Joback Method

Sources

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=R572957&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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