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
hfus	26.68	kJ/mol	Joback Method
logp	2.730		Crippen Method
mcvol	152.760	ml/mol	McGowan Method
rinpol	1734.00		NIST Webbook
rinpol	1734.00		NIST Webbook

Correlations

Information	Value
Property code	cpg
Equation	$Y = A + B \cdot T + C \cdot T^2 + D \cdot T^3 + E \cdot T.$
Y unit	J/mol×K
Coeff. A	-5.31980e+01
Coeff. B	1.15872e+00
Coeff. C	-8.59820e-04
Coeff. D	2.55800e-07
Coeff. E	0.00000e+00
Basis	predicted
Temperature range (K), min.	273.00
Temperature range (K), max.	1000.00

Information	Value
Property code	dvisc
Equation	Y = exp(A + B/T + C·ln(T) + D·T^E)
Y unit	Pa×s

Coeff. A	-9.10770e+00
Coeff. B	9.05660e+02
Coeff. C	0.00000e+00
Coeff. D	0.00000e+00
Coeff. E	0.00000e+00
Basis	predicted
Comment	Liquid phase. Joback/Reid (1987), valid from Tf to 0.7·Tc.
Temperature range (K), min.	328.33
Temperature range (K), max.	541.34

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R572957&Units=SI

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices

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