

trans-3n- butylidene phthalide

Inchi:	InChI=1S/C12H14O/c1-2-3-8-12-11-7-5-4-6-10(11)9-13-12/h4-8H,2-3,9H2,1H3/b12-8-
InchiKey:	QBNJDEITTLPXMW-WQLSENKSSA-N
Formula:	C12H14O
SMILES:	CCCC=C1OCc2ccccc21
Mol. weight [g/mol]:	174.24

Physical Properties

Property code	Value	Unit	Source
gf	180.74	kJ/mol	Joback Method
hf	-28.78	kJ/mol	Joback Method
hfus	25.85	kJ/mol	Joback Method
hvap	50.76	kJ/mol	Joback Method
log10ws	-3.91		Crippen Method
logp	3.358		Crippen Method
mcvol	146.890	ml/mol	McGowan Method
pc	2856.62	kPa	Joback Method
rinpol	1657.00		NIST Webbook
tb	550.62	K	Joback Method
tc	772.27	K	Joback Method
tf	323.05	K	Joback Method
vc	0.561	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	343.99	J/molxK	550.62	Joback Method
cpg	410.14	J/molxK	735.32	Joback Method
cpg	398.67	J/molxK	698.38	Joback Method
cpg	386.40	J/molxK	661.44	Joback Method
cpg	373.25	J/molxK	624.50	Joback Method
cpg	359.14	J/molxK	587.56	Joback Method
cpg	420.87	J/molxK	772.27	Joback Method
dvisc	0.0003646	Paxs	550.62	Joback Method
dvisc	0.0004325	Paxs	512.69	Joback Method

dvisc	0.0005271	Paxs	474.76	Joback Method
dvisc	0.0006650	Paxs	436.84	Joback Method
dvisc	0.0008767	Paxs	398.91	Joback Method
dvisc	0.0012251	Paxs	360.98	Joback Method
dvisc	0.0018518	Paxs	323.05	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=R219384&Units=SI

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

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