dibenzyl carbonate

Inchi: InChI=1S/C15H14O3/c16-15(17-11-13-7-3-1-4-8-13)18-12-14-9-5-2-6-10-14/h1-10H,11-1
InchiKey: PIZLBWGMERQCOC-UHFFFAOYSA-N
Formula: C15H14O3
SMILES: O=C(OCc1ccccc1)OCc1ccccc1
Mol. weight [g/mol]: 242.27
CAS: 3459-92-5

Physical Properties

Property code	Value	Unit	Source
gf	-38.68	kJ/mol	Joback Method
hf	-256.89	kJ/mol	Joback Method
hfus	26.66	kJ/mol	Joback Method
hvap	96.70 ± 0.70	kJ/mol	NIST Webbook
log10ws	-4.23		Crippen Method
logp	3.540		Crippen Method
mcvol	188.000	ml/mol	McGowan Method
pc	2584.59	kPa	Joback Method
tb	694.67	K	Joback Method
tc	928.83	K	Joback Method
tf	406.04	K	Joback Method
vc	0.702	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	567.17	J/mol×K	928.83	Joback Method
cpg	507.94	J/mol×K	733.70	Joback Method
cpg	522.05	J/mol×K	772.72	Joback Method
cpg	534.99	J/mol×K	811.75	Joback Method
cpg	546.80	J/mol×K	850.77	Joback Method
cpg	557.51	J/mol×K	889.80	Joback Method
cpg	492.63	J/mol×K	694.67	Joback Method
dvisc	0.0001362	Pa×s	646.56	Joback Method
dvisc	0.0001808	Pa×s	598.46	Joback Method

dvisc	0.0002523	Pa×s	550.36	Joback Method
dvisc	0.0003751	Pa×s	502.25	Joback Method
dvisc	0.0006067	Pa×s	454.14	Joback Method
dvisc	0.0001067	Pa×s	694.67	Joback Method
dvisc	0.0010998	Pa×s	406.04	Joback Method
pvap	1.03e-03	kPa	353.80	Vapour pressure and enthalpy of vaporization of aliphatic dialkyl carbonates
pvap	1.04e-03	kPa	354.20	Vapour pressure and enthalpy of vaporization of aliphatic dialkyl carbonates
pvap	1.29e-03	kPa	356.40	Vapour pressure and enthalpy of vaporization of aliphatic dialkyl carbonates
pvap	8.30e-04	kPa	351.20	Vapour pressure and enthalpy of vaporization of aliphatic dialkyl carbonates
pvap	1.73e-03	kPa	359.30	Vapour pressure and enthalpy of vaporization of aliphatic dialkyl carbonates
pvap	1.91e-03	kPa	361.50	Vapour pressure and enthalpy of vaporization of aliphatic dialkyl carbonates
pvap	2.20e-03	kPa	362.70	Vapour pressure and enthalpy of vaporization of aliphatic dialkyl carbonates
pvap	2.57e-03	kPa	364.30	Vapour pressure and enthalpy of vaporization of aliphatic dialkyl carbonates
pvap	3.27e-03	kPa	367.50	Vapour pressure and enthalpy of vaporization of aliphatic dialkyl carbonates
pvap	4.00e-03	kPa	369.60	Vapour pressure and enthalpy of vaporization of aliphatic dialkyl carbonates

pvap	3.99e-03	kPa	369.60	Vapour pressure and enthalpy of vaporization of aliphatic dialkyl carbonates
pvap	4.58e-03	kPa	371.60	Vapour pressure and enthalpy of vaporization of aliphatic dialkyl carbonates
pvap	5.22e-03	kPa	373.60	Vapour pressure and enthalpy of vaporization of aliphatic dialkyl carbonates
pvap	6.90e-04	kPa	349.20	Vapour pressure and enthalpy of vaporization of aliphatic dialkyl carbonates
pvap	6.80e-04	kPa	349.10	Vapour pressure and enthalpy of vaporization of aliphatic dialkyl carbonates
pvap	5.80e-04	kPa	346.70	Vapour pressure and enthalpy of vaporization of aliphatic dialkyl carbonates
pvap	4.90e-04	kPa	345.00	Vapour pressure and enthalpy of vaporization of aliphatic dialkyl carbonates
pvap	4.90e-04	kPa	344.80	Vapour pressure and enthalpy of vaporization of aliphatic dialkyl carbonates
pvap	3.60e-04	kPa	341.70	Vapour pressure and enthalpy of vaporization of aliphatic dialkyl carbonates
pvap	1.68e-03	kPa	359.20	Vapour pressure and enthalpy of vaporization of aliphatic dialkyl carbonates

Sources

Vapour pressure and enthalpy of vaporization of aliphatic dialkyl carbonates:	https://www.doi.org/10.1016/j.jct.2008.02.012
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=C3459925&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume