

Ethyl 3-phenoxybenzyl carbonate

Inchi:	InChI=1S/C16H16O4/c1-2-18-16(17)19-12-13-7-6-10-15(11-13)20-14-8-4-3-5-9-14/h3-11
InchiKey:	QWZOIUHCSRTKRV-UHFFFAOYSA-N
Formula:	C16H16O4
SMILES:	CCOC(=O)OCc1cccc(Oc2ccccc2)c1
Mol. weight [g/mol]:	272.30

Physical Properties

Property code	Value	Unit	Source
gf	-144.89	kJ/mol	Joback Method
hf	-421.22	kJ/mol	Joback Method
hfus	30.05	kJ/mol	Joback Method
hvap	70.40	kJ/mol	Joback Method
log10ws	-4.17		Crippen Method
logp	4.152		Crippen Method
mcvol	207.960	ml/mol	McGowan Method
pc	2278.41	kPa	Joback Method
rinpol	2069.00		NIST Webbook
tb	744.95	K	Joback Method
tc	972.58	K	Joback Method
tf	452.06	K	Joback Method
vc	0.775	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	570.98	J/mol×K	744.95	Joback Method
cpg	585.99	J/mol×K	782.89	Joback Method
cpg	599.81	J/mol×K	820.83	Joback Method
cpg	612.44	J/mol×K	858.76	Joback Method
cpg	623.89	J/mol×K	896.70	Joback Method
cpg	634.18	J/mol×K	934.64	Joback Method
cpg	643.32	J/mol×K	972.58	Joback Method
dvisc	0.0006153	Paxs	452.06	Joback Method
dvisc	0.0003632	Paxs	500.88	Joback Method

dvisc	0.0002354	Paxs	549.69	Joback Method
dvisc	0.0001638	Paxs	598.50	Joback Method
dvisc	0.0001204	Paxs	647.32	Joback Method
dvisc	0.0000924	Paxs	696.13	Joback Method
dvisc	0.0000734	Paxs	744.95	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U373802&Units=SI
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

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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