

BUTYL PENTYL CARBONATE

Inchi:	InChI=1S/C10H20O3/c1-3-5-7-9-13-10(11)12-8-6-4-2/h3-9H2,1-2H3
InchiKey:	FLIHROUXKOLBTC-UHFFFAOYSA-N
Formula:	C10H20O3
SMILES:	CCCCCOC(=O)OCCCC
Mol. weight [g/mol]:	188.27

Physical Properties

Property code	Value	Unit	Source
af	0.6752		Cheméo Relay (1.0)
gf	-305.60	kJ/mol	Joback Method
hf	-734.66	kJ/mol	Cheméo Relay (1.0)
hfus	25.63	kJ/mol	Joback Method
hvap	67.69	kJ/mol	Cheméo Relay (1.0)
ie	10.04	eV	Cheméo Relay (1.0)
log10ws	-3.27		Cheméo Relay (1.0)
logp	3.130		Crippen Method
mcvol	165.070	ml/mol	McGowan Method
pc	2165.35	kPa	Joback Method
tb	490.10	K	Cheméo Relay (1.0)
tc	638.44	K	Cheméo Relay (1.0)
tf	206.84	K	Cheméo Relay (1.0)
vc	0.650	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	394.21	J/mol×K	526.91	Joback Method
cpg	408.16	J/mol×K	555.55	Joback Method
cpg	421.63	J/mol×K	584.18	Joback Method
cpg	434.61	J/mol×K	612.82	Joback Method
cpg	447.09	J/mol×K	641.45	Joback Method
cpg	459.09	J/mol×K	670.09	Joback Method
cpg	470.59	J/mol×K	698.72	Joback Method
dvisc	0.0023638	Pa×s	296.85	Joback Method

dvisc	0.0012078	Pa×s	335.19	Joback Method
dvisc	0.0007084	Pa×s	373.54	Joback Method
dvisc	0.0004589	Pa×s	411.88	Joback Method
dvisc	0.0003200	Pa×s	450.22	Joback Method
dvisc	0.0002362	Pa×s	488.57	Joback Method
dvisc	0.0001822	Pa×s	526.91	Joback Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C83073034&Units=SI>

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):

Legend

af:	Acentric Factor
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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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