CYCLOHEXANOL, 2-BUTYL-

Inchi: InChI=1S/C10H20O/c1-2-3-6-9-7-4-5-8-10(9)11/h9-11H,2-8H2,1H3
InchiKey: LVDALGYBEFALAP-UHFFFAOYSA-N
Formula: C10H20O
SMILES: CCCCC1CCCCC1O
Mol. weight [g/mol]: 156.27

Physical Properties

Property code	Value	Unit	Source
af	0.5587		Cheméo Relay (1.0)
gf	-86.76	kJ/mol	Joback Method
hf	-352.69	kJ/mol	Cheméo Relay (1.0)
hfus	18.65	kJ/mol	Joback Method
hvap	74.62	kJ/mol	Cheméo Relay (1.0)
ie	9.59	eV	Cheméo Relay (1.0)
log10ws	-2.95		Cheméo Relay (1.0)
logp	2.728		Crippen Method
mcvol	146.770	ml/mol	McGowan Method
pc	2729.71	kPa	Joback Method
tb	498.14	K	Cheméo Relay (1.0)
tc	702.40	K	Cheméo Relay (1.0)
tf	266.60	K	Cheméo Relay (1.0)
vc	0.520	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	369.43	J/mol×K	535.26	Joback Method
cpg	458.23	J/mol×K	721.21	Joback Method
cpg	445.27	J/mol×K	690.22	Joback Method
cpg	431.60	J/mol×K	659.23	Joback Method
cpg	417.20	J/mol×K	628.24	Joback Method
cpg	402.05	J/mol×K	597.24	Joback Method
cpg	386.13	J/mol×K	566.25	Joback Method
dvisc	0.0008187	Pa×s	400.84	Joback Method

dvisc	0.0001375	Pa×s	535.26	Joback Method
dvisc	0.0002235	Pa×s	490.45	Joback Method
dvisc	0.0004007	Pa×s	445.65	Joback Method
dvisc	0.0295183	Pa×s	266.42	Joback Method
dvisc	0.0020021	Pa×s	356.03	Joback Method
dvisc	0.0063338	Pa×s	311.23	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C36159496&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

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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