4-CYCLOHEXYL-1-BUTANOL

Other names:	Cyclohexanebutanol- cyclohexylbutan-1-ol
Inchi:	InChI=1S/C10H20O/c11-9-5-4-8-10-6-2-1-3-7-10/h10-11H,1-9H2
InchiKey:	NZEBWPHHIQAVOH-UHFFFAOYSA-N
Formula:	C10H20O
SMILES:	OCCCCC1CCCCC1
Mol. weight [g/mol]:	156.27

Physical Properties

Property code	Value	Unit	Source
af	0.6602		Cheméo Relay (1.0)
gf	-79.05	kJ/mol	Joback Method
hf	-362.08	kJ/mol	Cheméo Relay (1.0)
hfus	17.58	kJ/mol	Joback Method
hvap	78.13	kJ/mol	Cheméo Relay (1.0)
ie	9.77	eV	Cheméo Relay (1.0)
log10ws	-3.13		Cheméo Relay (1.0)
logp	2.729		Crippen Method
mcvol	146.770	ml/mol	McGowan Method
pc	2826.33	kPa	Joback Method
tb	527.42	K	Cheméo Relay (1.0)
tc	744.32	K	Cheméo Relay (1.0)
tf	272.00	K	Cheméo Relay (1.0)
vc	0.508	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	368.65	J/mol×K	539.93	Joback Method
cpg	384.97	J/mol×K	570.96	Joback Method
cpg	400.50	J/mol×K	601.99	Joback Method
cpg	415.25	J/mol×K	633.03	Joback Method
cpg	429.25	J/mol×K	664.06	Joback Method
cpg	442.52	J/mol×K	695.09	Joback Method

cpg	455.09	J/mol×K	726.12	Joback Method
dvisc	0.0367328	Pa×s	270.66	Joback Method
dvisc	0.0072198	Pa×s	315.54	Joback Method
dvisc	0.0021279	Pa×s	360.42	Joback Method
dvisc	0.0008220	Pa×s	405.30	Joback Method
dvisc	0.0003838	Pa×s	450.17	Joback Method
dvisc	0.0002058	Pa×s	495.05	Joback Method
dvisc	0.0001224	Pa×s	539.93	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	376.70	K	0.50	NIST Webbook

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C4441570&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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume