

Cyclohexanecarboxylic acid, butyl ester

Other names:	butyl cyclohexanecarboxylate
Inchi:	InChI=1S/C11H20O2/c1-2-3-9-13-11(12)10-7-5-4-6-8-10/h10H,2-9H2,1H3
InchiKey:	IPGMIYAOWRJGBE-UHFFFAOYSA-N
Formula:	C11H20O2
SMILES:	CCCCOC(=O)C1CCCCC1
Mol. weight [g/mol]:	184.28
CAS:	6553-81-7

Physical Properties

Property code	Value	Unit	Source
gf	-167.73	kJ/mol	Joback Method
hf	-460.85	kJ/mol	Joback Method
hfus	18.87	kJ/mol	Joback Method
hvap	49.67	kJ/mol	Joback Method
log10ws	-2.94		Crippen Method
logp	2.910		Crippen Method
mcvol	162.430	ml/mol	McGowan Method
pc	2443.48	kPa	Joback Method
rinpol	1305.46		NIST Webbook
rinpol	1305.46		NIST Webbook
rinpol	1309.75		NIST Webbook
tb	546.92	K	Joback Method
tc	749.25	K	Joback Method
tf	293.27	K	Joback Method
vc	0.609	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	404.06	J/molxK	546.92	Joback Method
cpg	422.58	J/molxK	580.64	Joback Method
cpg	440.17	J/molxK	614.36	Joback Method
cpg	456.83	J/molxK	648.08	Joback Method
cpg	472.58	J/molxK	681.81	Joback Method

cpg	487.44	J/molxK	715.53	Joback Method
cpg	501.43	J/molxK	749.25	Joback Method
dvisc	0.0040594	Paxs	293.27	Joback Method
dvisc	0.0018425	Paxs	335.54	Joback Method
dvisc	0.0009979	Paxs	377.82	Joback Method
dvisc	0.0006115	Paxs	420.09	Joback Method
dvisc	0.0004098	Paxs	462.37	Joback Method
dvisc	0.0002937	Paxs	504.64	Joback Method
dvisc	0.0002216	Paxs	546.92	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6553817&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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