Butanoic acid, cyclohexyl ester

Other names:	Butyric acid, cyclohexyl ester
	Cyclohexanol butanoate
	Cyclohexanyl butyrate
	Cyclohexyl butyrate
	Cyclohexyl n-butyrate
	cyclohexyl butanoate
	n-Butyric acid cyclohexyl ester
Inchi:	InChI=1S/C10H18O2/c1-2-6-10(11)12-9-7-4-3-5-8-9/h9H,2-8H2,1H3
InchiKey:	VZHUBBUZNIULNM-UHFFFAOYSA-N
Formula:	C10H18O2
SMILES:	CCCC(=O)OC1CCCCC1
Mol. weight [g/mol]:	170.25
CAS:	1551-44-6

Physical Properties

Property code	Value	Unit	Source
chl	-5912.40 ± 2.70	kJ/mol	NIST Webbook
gf	-176.15	kJ/mol	Joback Method
hf	-545.70 ± 2.80	kJ/mol	NIST Webbook
hfl	-605.70 ± 2.70	kJ/mol	NIST Webbook
hfus	16.28	kJ/mol	Joback Method
hvap	64.10 ± 0.60	kJ/mol	NIST Webbook
hvap	60.00 ± 0.60	kJ/mol	NIST Webbook
hvap	60.00	kJ/mol	NIST Webbook
hvap	60.04 ± 0.63	kJ/mol	NIST Webbook
hvap	60.00	kJ/mol	NIST Webbook
hvap	58.40 ± 0.70	kJ/mol	NIST Webbook
hvap	59.80 ± 0.60	kJ/mol	NIST Webbook
hvap	60.00 ± 0.20	kJ/mol	NIST Webbook
hvap	60.10 ± 0.20	kJ/mol	NIST Webbook
log10ws	-2.88		Crippen Method
logp	2.662		Crippen Method
mcvol	148.340	ml/mol	McGowan Method
pc	2693.00	kPa	Joback Method
rinpol	1209.00		NIST Webbook
rinpol	1202.00		NIST Webbook
rinpol	1209.00		NIST Webbook

ripol	1492.00		NIST Webbook
tb	524.04	K	Joback Method
tc	729.39	K	Joback Method
tf	282.00	K	Joback Method
tt	219.60 ± 0.15	K	NIST Webbook
vc	0.552	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	355.31	J/mol×K	524.04	Joback Method
cpg	373.16	J/mol×K	558.27	Joback Method
cpg	390.11	J/mol×K	592.49	Joback Method
cpg	406.18	J/mol×K	626.72	Joback Method
cpg	421.39	J/mol×K	660.94	Joback Method
cpg	435.73	J/mol×K	695.17	Joback Method
cpg	449.24	J/mol×K	729.39	Joback Method
dvisc	0.0042103	Pa×s	282.00	Joback Method
dvisc	0.0019412	Pa×s	322.34	Joback Method
dvisc	0.0010632	Pa×s	362.68	Joback Method
dvisc	0.0006569	Pa×s	403.02	Joback Method
dvisc	0.0004431	Pa×s	443.36	Joback Method
dvisc	0.0003191	Pa×s	483.70	Joback Method
dvisc	0.0002418	Pa×s	524.04	Joback Method
hvapt	58.72	kJ/mol	315.57	Comprehensive Study of Vapor Pressures and Enthalpies of Vaporization of Cyclohexyl Esters

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Comprehensive Study of Vapor Pressures and Enthalpies of Vaporization of Cyclohexyl Esters: https://www.doi.org/10.1021/je025634v

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1551446&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume