Pentanoic acid, cyclohexyl ester

Other names:	1-Cyclohexyl pentanoate
	cyclohexyl pentanoate
	cyclohexyl valerate
	valeric acid, cyclohexyl ester
Inchi:	InChI=1S/C11H20O2/c1-2-3-9-11(12)13-10-7-5-4-6-8-10/h10H,2-9H2,1H3
InchiKey:	YLCHTSSXNSNXSW-UHFFFAOYSA-N
Formula:	C11H20O2
SMILES:	CCCCC(=O)OC1CCCCC1
Mol. weight [g/mol]:	184.28
CAS:	1551-43-5

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	62.40 ± 0.70	kJ/mol	NIST Webbook
hvap	63.70 ± 0.10	kJ/mol	NIST Webbook
hvap	63.90 ± 0.40	kJ/mol	NIST Webbook
hvap	67.20 ± 0.80	kJ/mol	NIST Webbook
log10ws	-3.30		Crippen Method
logp	3.053		Crippen Method
mcvol	162.430	ml/mol	McGowan Method
pc	2443.48	kPa	Joback Method
rinpol	1310.00		NIST Webbook
rinpol	1299.00		NIST Webbook
ripol	1595.00		NIST Webbook
tb	546.92	K	Joback Method
tc	749.25	K	Joback Method
tf	293.27	K	Joback Method
tt	222.40 ± 0.15	K	NIST Webbook
vc	0.609	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	404.06	J/mol×K	546.92	Joback Method
cpg	422.58	J/mol×K	580.64	Joback Method
cpg	440.17	J/mol×K	614.36	Joback Method
cpg	456.83	J/mol×K	648.08	Joback Method
cpg	472.58	J/mol×K	681.81	Joback Method
cpg	487.44	J/mol×K	715.53	Joback Method
cpg	501.43	J/mol×K	749.25	Joback Method
dvisc	0.0040594	Pa×s	293.27	Joback Method
dvisc	0.0018425	Pa×s	335.54	Joback Method
dvisc	0.0009979	Pa×s	377.82	Joback Method
dvisc	0.0006115	Pa×s	420.09	Joback Method
dvisc	0.0004098	Pa×s	462.37	Joback Method
dvisc	0.0002937	Pa×s	504.64	Joback Method
dvisc	0.0002216	Pa×s	546.92	Joback Method
hvapt	63.60	kJ/mol	299.54	Comprehensive Study of Vapor Pressures and Enthalpies of Vaporization of Cyclohexyl Esters

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1551435&Units=SI

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

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

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
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