

Valeric acid, 4-chlorophenyl ester

Inchi:	InChI=1S/C11H13ClO2/c1-2-3-4-11(13)14-10-7-5-9(12)6-8-10/h5-8H,2-4H2,1H3
InchiKey:	BEZFOOVQBIWCMU-UHFFFAOYSA-N
Formula:	C11H13ClO2
SMILES:	CCCCC(=O)Oc1ccc(Cl)cc1
Mol. weight [g/mol]:	212.67

Physical Properties

Property code	Value	Unit	Source
gf	-101.33	kJ/mol	Joback Method
hf	-305.85	kJ/mol	Joback Method
hfus	24.88	kJ/mol	Joback Method
hvap	56.56	kJ/mol	Joback Method
log10ws	-3.73		Crippen Method
logp	3.436		Crippen Method
mvol	161.770	ml/mol	McGowan Method
pc	2632.55	kPa	Joback Method
rinpol	1510.00		NIST Webbook
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tb	596.46	K	Joback Method
tc	810.87	K	Joback Method
tf	354.75	K	Joback Method
vc	0.617	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	372.82	J/mol×K	596.46	Joback Method
cpg	386.14	J/mol×K	632.19	Joback Method
cpg	398.67	J/mol×K	667.93	Joback Method
cpg	410.44	J/mol×K	703.66	Joback Method
cpg	421.46	J/mol×K	739.40	Joback Method
cpg	431.76	J/mol×K	775.13	Joback Method
cpg	441.35	J/mol×K	810.87	Joback Method
dvisc	0.0016178	Paxs	354.75	Joback Method

dvisc	0.0009457	Paxs	395.04	Joback Method
dvisc	0.0006105	Paxs	435.32	Joback Method
dvisc	0.0004245	Paxs	475.61	Joback Method
dvisc	0.0003124	Paxs	515.89	Joback Method
dvisc	0.0002403	Paxs	556.17	Joback Method
dvisc	0.0001915	Paxs	596.46	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307984&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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
mccvol:	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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