

Valeric acid, pentadecyl ester

Inchi:	InChI=1S/C20H40O2/c1-3-5-7-8-9-10-11-12-13-14-15-16-17-19-22-20(21)18-6-4-2/h3-19
InchiKey:	ZDYLNFIQQYOU MX-UHFFFAOYSA-N
Formula:	C20H40O2
SMILES:	CCCCCCCCCCCCCCCCOC(=O)CCCC
Mol. weight [g/mol]:	312.53
CAS:	125164-53-6

Physical Properties

Property code	Value	Unit	Source
gf	-116.40	kJ/mol	Joback Method
hf	-700.93	kJ/mol	Joback Method
hfus	50.34	kJ/mol	Joback Method
hvap	69.27	kJ/mol	Joback Method
log10ws	-7.06		Crippen Method
logp	6.811		Crippen Method
mcvol	300.100	ml/mol	McGowan Method
pc	1045.97	kPa	Joback Method
tb	733.29	K	Joback Method
tc	904.52	K	Joback Method
tf	387.32	K	Joback Method
vc	1.179	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	908.52	J/mol×K	733.29	Joback Method
cpg	928.17	J/mol×K	761.83	Joback Method
cpg	946.91	J/mol×K	790.37	Joback Method
cpg	964.76	J/mol×K	818.91	Joback Method
cpg	981.74	J/mol×K	847.45	Joback Method
cpg	997.86	J/mol×K	875.99	Joback Method
cpg	1013.17	J/mol×K	904.52	Joback Method
dvisc	0.0016619	Pa×s	387.32	Joback Method
dvisc	0.0007053	Pa×s	444.98	Joback Method

dvisc	0.0003644	Pa×s	502.64	Joback Method
dvisc	0.0002156	Pa×s	560.30	Joback Method
dvisc	0.0001407	Pa×s	617.97	Joback Method
dvisc	0.0000988	Pa×s	675.63	Joback Method
dvisc	0.0000733	Pa×s	733.29	Joback Method

Sources

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=C125164536&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:

<https://www.chemeo.com/cid/26-852-7/Valeric-acid-pentadecyl-ester.pdf>

Generated by Cheméo on 2025-12-05 20:08:42.986201155 +0000 UTC m=+4713520.516241809.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.