

Valeric acid, tridecyl ester

Inchi:	InChI=1S/C18H36O2/c1-3-5-7-8-9-10-11-12-13-14-15-17-20-18(19)16-6-4-2/h3-17H2,1-2
InchiKey:	KGUAWIPVMCVZCA-UHFFFAOYSA-N
Formula:	C18H36O2
SMILES:	CCCCCCCCCCCCOC(=O)CCCC
Mol. weight [g/mol]:	284.48
CAS:	117177-34-1

Physical Properties

Property code	Value	Unit	Source
gf	-133.24	kJ/mol	Joback Method
hf	-659.65	kJ/mol	Joback Method
hfus	45.16	kJ/mol	Joback Method
hvap	64.82	kJ/mol	Joback Method
log10ws	-6.22		Crippen Method
logp	6.031		Crippen Method
mcvol	271.920	ml/mol	McGowan Method
pc	1189.06	kPa	Joback Method
tb	687.53	K	Joback Method
tc	855.83	K	Joback Method
tf	364.78	K	Joback Method
vc	1.067	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	789.92	J/molxK	687.53	Joback Method
cpg	875.72	J/molxK	827.78	Joback Method
cpg	860.14	J/molxK	799.73	Joback Method
cpg	843.80	J/molxK	771.68	Joback Method
cpg	826.65	J/molxK	743.63	Joback Method
cpg	808.70	J/molxK	715.58	Joback Method
cpg	890.54	J/molxK	855.83	Joback Method
dvisc	0.0000953	Paxs	687.53	Joback Method
dvisc	0.0001278	Paxs	633.74	Joback Method

dvisc	0.0001809	Paxs	579.95	Joback Method
dvisc	0.0002749	Paxs	526.15	Joback Method
dvisc	0.0004595	Paxs	472.36	Joback Method
dvisc	0.0008765	Paxs	418.57	Joback Method
dvisc	0.0020226	Paxs	364.78	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C117177341&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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

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