

Dodecanoic acid, 2-methylpentyl ester

Inchi:	InChI=1S/C18H36O2/c1-4-6-7-8-9-10-11-12-13-15-18(19)20-16-17(3)14-5-2/h17H,4-16H
InchiKey:	AGSWKPMKNYLPHP-UHFFFAOYSA-N
Formula:	C18H36O2
SMILES:	CCCCCCCCCCCC(=O)OCC(C)CCC
Mol. weight [g/mol]:	284.48

Physical Properties

Property code	Value	Unit	Source
gf	-135.68	kJ/mol	Joback Method
hf	-664.93	kJ/mol	Joback Method
hfus	41.64	kJ/mol	Joback Method
hvap	64.43	kJ/mol	Joback Method
log10ws	-5.98		Crippen Method
logp	5.887		Crippen Method
mcvol	271.920	ml/mol	McGowan Method
pc	1195.65	kPa	Joback Method
rinsol	1956.00		NIST Webbook
tb	687.09	K	Joback Method
tc	857.14	K	Joback Method
tf	349.78	K	Joback Method
vc	1.062	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	790.33	J/molxK	687.09	Joback Method
cpg	877.02	J/molxK	828.80	Joback Method
cpg	861.31	J/molxK	800.46	Joback Method
cpg	844.81	J/molxK	772.12	Joback Method
cpg	827.49	J/molxK	743.77	Joback Method
cpg	809.34	J/molxK	715.43	Joback Method
cpg	891.94	J/molxK	857.14	Joback Method
dvisc	0.0000883	Paxs	687.09	Joback Method
dvisc	0.0001207	Paxs	630.87	Joback Method

dvisc	0.0001755	Paxs	574.65	Joback Method
dvisc	0.0002766	Paxs	518.43	Joback Method
dvisc	0.0004870	Paxs	462.22	Joback Method
dvisc	0.0010029	Paxs	406.00	Joback Method
dvisc	0.0026053	Paxs	349.78	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U360542&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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