2-Ethylbutyric acid, dodecyl ester

Inchi: InChI=1S/C18H36O2/c1-4-7-8-9-10-11-12-13-14-15-16-20-18(19)17(5-2)6-3/h17H,4-16H
InchiKey: NOZDRKNOMKZEFU-UHFFFAOYSA-N
Formula: C18H36O2
SMILES: CCCCCCCCCCCCOC(=O)C(CC)CC
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
rinpol	1874.00		NIST Webbook
rinpol	1874.00		NIST Webbook
rinpol	1915.00		NIST Webbook
rinpol	1915.00		NIST Webbook
tb	687.09	K	Joback Method
tc	857.14	K	Joback Method
tf	349.78	K	Joback Method
vc	1.062	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	790.33	J/mol×K	687.09	Joback Method
cpg	877.02	J/mol×K	828.80	Joback Method
cpg	861.31	J/mol×K	800.46	Joback Method
cpg	844.81	J/mol×K	772.12	Joback Method
cpg	827.49	J/mol×K	743.77	Joback Method
cpg	809.34	J/mol×K	715.43	Joback Method

cpg	891.94	J/mol×K	857.14	Joback Method
dvisc	0.0000883	Pa×s	687.09	Joback Method
dvisc	0.0001207	Pa×s	630.87	Joback Method
dvisc	0.0001755	Pa×s	574.65	Joback Method
dvisc	0.0002766	Pa×s	518.43	Joback Method
dvisc	0.0004870	Pa×s	462.22	Joback Method
dvisc	0.0010029	Pa×s	406.00	Joback Method
dvisc	0.0026053	Pa×s	349.78	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=U369723&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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