ISOBUTYL MYRISTATE

Other names: Tetradecanoic acid, 2-methylpropyl ester
2-methylpropyl tetradecanoate
Isobutyl myristate
Inchi: InChI=1S/C18H36O2/c1-4-5-6-7-8-9-10-11-12-13-14-15-18(19)20-16-17(2)3/h17H,4-16H
InchiKey: SKVCWXRLKHBEKW-UHFFFAOYSA-N
Formula: C18H36O2
SMILES: CCCCCCCCCCCCCC(=O)OCC(C)C
Mol. weight [g/mol]: 284.48

Physical Properties

Property code	Value	Unit	Source
af	0.8771		Cheméo Relay (1.0)
hf	-742.37	kJ/mol	Cheméo Relay (1.0)
hfus	41.64	kJ/mol	Joback Method
hvap	85.41	kJ/mol	Cheméo Relay (1.0)
ie	9.70	eV	Cheméo Relay (1.0)
log10ws	-6.18		Cheméo Relay (1.0)
logp	5.887		Crippen Method
mcvol	271.920	ml/mol	McGowan Method
pc	1195.65	kPa	Joback Method
rinpol	1914.00		NIST Webbook
rinpol	1950.00		NIST Webbook
rinpol	1927.00		NIST Webbook
rinpol	1927.00		NIST Webbook
rinpol	1950.00		NIST Webbook
ripol	2160.00		NIST Webbook
ripol	2160.00		NIST Webbook
tb	577.69	K	Cheméo Relay (1.0)
tc	747.89	K	Cheméo Relay (1.0)
tf	274.35	K	Cheméo Relay (1.0)
vc	1.060	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	790.33	J/mol×K	687.09	Joback Method
cpg	891.94	J/mol×K	857.14	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
dvisc	0.0002766	Pa×s	518.43	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	0.0026053	Pa×s	349.78	Joback Method
dvisc	0.0004870	Pa×s	462.22	Joback Method
dvisc	0.0010029	Pa×s	406.00	Joback Method

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C25263972&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

af: Acentric Factor
cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hvap: Enthalpy of vaporization at standard conditions
ie: Ionization energy
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume