3-methylbutyl hexadecanoate

Other names: isopentyl hexadecanoate
3-methylbutyl palmitate
Inchi: InChI=1S/C21H42O2/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-21(22)23-19-18-20(2)3/h2
InchiKey: NXBIDOXPIIWDMX-UHFFFAOYSA-N
Formula: C21H42O2
SMILES: CCCCCCCCCCCCCCCC(=O)OCCC(C)C
Mol. weight [g/mol]: 326.56
CAS: 81974-61-0

Physical Properties

Property code	Value	Unit	Source
gf	-110.42	kJ/mol	Joback Method
hf	-726.85	kJ/mol	Joback Method
hfus	49.41	kJ/mol	Joback Method
hvap	71.11	kJ/mol	Joback Method
log10ws	-7.23		Crippen Method
logp	7.057		Crippen Method
mcvol	314.190	ml/mol	McGowan Method
pc	988.88	kPa	Joback Method
rinpol	2246.00		NIST Webbook
rinpol	2246.00		NIST Webbook
rinpol	2260.00		NIST Webbook
rinpol	2260.00		NIST Webbook
ripol	2479.00		NIST Webbook
ripol	2479.00		NIST Webbook
tb	755.73	K	Joback Method
tc	930.28	K	Joback Method
tf	383.59	K	Joback Method
vc	1.230	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	969.75	J/mol×K	755.73	Joback Method

cpg	1061.34	J/mol×K	901.19	Joback Method
cpg	1044.89	J/mol×K	872.09	Joback Method
cpg	1027.53	J/mol×K	843.00	Joback Method
cpg	1009.24	J/mol×K	813.91	Joback Method
cpg	989.99	J/mol×K	784.82	Joback Method
cpg	1076.91	J/mol×K	930.28	Joback Method
dvisc	0.0000590	Pa×s	755.73	Joback Method
dvisc	0.0000811	Pa×s	693.71	Joback Method
dvisc	0.0001187	Pa×s	631.68	Joback Method
dvisc	0.0001889	Pa×s	569.66	Joback Method
dvisc	0.0003366	Pa×s	507.64	Joback Method
dvisc	0.0007045	Pa×s	445.61	Joback Method
dvisc	0.0018724	Pa×s	383.59	Joback Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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=C81974610&Units=SI

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

ripol: Polar retention indices

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/80-230-7/3-methylbutyl-hexadecanoate.pdf
Generated by Cheméo on 2024-04-17 15:16:25.232916667 +0000 UTC m=+15656234.153493979.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.