

Methyl 18-methylnonadecanoate

Inchi:

InChI=1S/C21H42O2/c1-20(2)18-16-14-12-10-8-6-4-5-7-9-11-13-15-17-19-21(22)23-3/h2

InchiKey:

IVHQIMJNEKWLSS-UHFFFAOYSA-N

Formula:

C21H42O2

SMILES:

COC(=O)CCCCCCCCCCCCCCCCC(C)C

Mol. weight [g/mol]:

326.56

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	2290.80		NIST Webbook
rinpol	2277.00		NIST Webbook
rinpol	2277.00		NIST Webbook
rinpol	2290.80		NIST Webbook
rinpol	2277.00		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/molxK	755.73	Joback Method
cpg	989.99	J/molxK	784.82	Joback Method
cpg	1009.24	J/molxK	813.91	Joback Method
cpg	1027.53	J/molxK	843.00	Joback Method
cpg	1044.89	J/molxK	872.09	Joback Method

cpg	1061.34	J/molxK	901.19	Joback Method
cpg	1076.91	J/molxK	930.28	Joback Method
dvisc	0.0018724	Paxs	383.59	Joback Method
dvisc	0.0007045	Paxs	445.61	Joback Method
dvisc	0.0003366	Paxs	507.64	Joback Method
dvisc	0.0001889	Paxs	569.66	Joback Method
dvisc	0.0001187	Paxs	631.68	Joback Method
dvisc	0.0000811	Paxs	693.71	Joback Method
dvisc	0.0000590	Paxs	755.73	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U352206&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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

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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