

n-Propyl heptadecanoate

Other names:	propyl heptadecanoate
Inchi:	InChI=1S/C20H40O2/c1-3-5-6-7-8-9-10-11-12-13-14-15-16-17-18-20(21)22-19-4-2/h3-19
InchiKey:	SXTULBAGGXUEQH-UHFFFAOYSA-N
Formula:	C20H40O2
SMILES:	CCCCCCCCCCCCCCCC(=O)OCCC
Mol. weight [g/mol]:	312.53

Physical Properties

Property code	Value	Unit	Source
gf	-116.40	kJ/mol	Joback Method
hf	-700.93	kJ/mol	Joback Method
hfus	50.34	kJ/mol	Joback Method
hvap	69.27	kJ/mol	Joback Method
log10ws	-7.06		Crippen Method
logp	6.811		Crippen Method
mcvol	300.100	ml/mol	McGowan Method
pc	1045.97	kPa	Joback Method
rinpol	2172.00		NIST Webbook
rinpol	2193.00		NIST Webbook
rinpol	2193.00		NIST Webbook
rinpol	2172.00		NIST Webbook
tb	733.29	K	Joback Method
tc	904.52	K	Joback Method
tf	387.32	K	Joback Method
vc	1.179	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	908.52	J/molxK	733.29	Joback Method
cpg	928.17	J/molxK	761.83	Joback Method
cpg	946.91	J/molxK	790.37	Joback Method
cpg	964.76	J/molxK	818.91	Joback Method
cpg	981.74	J/molxK	847.45	Joback Method

cpg	997.86	J/mol×K	875.99	Joback Method
cpg	1013.17	J/mol×K	904.52	Joback Method
dvisc	0.0016619	Paxs	387.32	Joback Method
dvisc	0.0007053	Paxs	444.98	Joback Method
dvisc	0.0003644	Paxs	502.64	Joback Method
dvisc	0.0002156	Paxs	560.30	Joback Method
dvisc	0.0001407	Paxs	617.97	Joback Method
dvisc	0.0000988	Paxs	675.63	Joback Method
dvisc	0.0000733	Paxs	733.29	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U336683&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
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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