

1-Heneicosyl formate

Inchi:	InChI=1S/C22H44O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-24-22-23
InchiKey:	ZMGJNJFHZNMCW-UHFFFAOYSA-N
Formula:	C22H44O2
SMILES:	CCCCCCCCCCCCCCCCCCCCOC=O
Mol. weight [g/mol]:	340.58
CAS:	77899-03-7

Physical Properties

Property code	Value	Unit	Source
gf	-70.16	kJ/mol	Joback Method
hf	-715.21	kJ/mol	Joback Method
hfus	56.21	kJ/mol	Joback Method
hvap	73.70	kJ/mol	Joback Method
log10ws	-7.89		Crippen Method
logp	7.591		Crippen Method
mcvol	328.280	ml/mol	McGowan Method
pc	933.49	kPa	Joback Method
tb	773.84	K	Joback Method
tc	948.88	K	Joback Method
tf	401.93	K	Joback Method
vc	1.302	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1029.43	J/molxK	773.84	Joback Method
cpg	1122.22	J/molxK	919.70	Joback Method
cpg	1105.55	J/molxK	890.53	Joback Method
cpg	1087.96	J/molxK	861.36	Joback Method
cpg	1069.43	J/molxK	832.19	Joback Method
cpg	1049.93	J/molxK	803.01	Joback Method
cpg	1138.00	J/molxK	948.88	Joback Method
dvisc	0.0000622	Paxs	773.84	Joback Method
dvisc	0.0000843	Paxs	711.85	Joback Method

dvisc	0.0001210	Paxs	649.87	Joback Method
dvisc	0.0001874	Paxs	587.88	Joback Method
dvisc	0.0003218	Paxs	525.90	Joback Method
dvisc	0.0006385	Paxs	463.91	Joback Method
dvisc	0.0015648	Paxs	401.93	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=C77899037&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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