

1,1-Nonadecanedicarboxylic acid

Other names:	octadecylmalonic acid
Inchi:	InChI=1S/C21H40O4/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19(20(22)23)21(24)
InchiKey:	WMUFHDYXFASDAE-UHFFFAOYSA-N
Formula:	C21H40O4
SMILES:	CCCCCCCCCCCCCCCCCCC(C(=O)O)C(=O)O
Mol. weight [g/mol]:	356.54
CAS:	4475-04-1

Physical Properties

Property code	Value	Unit	Source
gf	-407.98	kJ/mol	Joback Method
hf	-1011.67	kJ/mol	Joback Method
hfus	58.00	kJ/mol	Joback Method
hvap	108.80	kJ/mol	Joback Method
log10ws	-6.57		Crippen Method
logp	6.423		Crippen Method
mcvol	321.630	ml/mol	McGowan Method
pc	1176.05	kPa	Joback Method
tb	971.54	K	Joback Method
tc	1202.31	K	Joback Method
tf	532.93	K	Joback Method
vc	1.256	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1105.63	J/molxK	971.54	Joback Method
cpg	1123.07	J/molxK	1010.00	Joback Method
cpg	1139.27	J/molxK	1048.46	Joback Method
cpg	1154.32	J/molxK	1086.92	Joback Method
cpg	1168.29	J/molxK	1125.38	Joback Method
cpg	1181.26	J/molxK	1163.84	Joback Method
cpg	1193.33	J/molxK	1202.31	Joback Method
dvisc	0.0002452	Paxs	532.93	Joback Method

dvisc	0.0000595	Paxs	606.03	Joback Method
dvisc	0.0000196	Paxs	679.13	Joback Method
dvisc	0.0000080	Paxs	752.24	Joback Method
dvisc	0.0000038	Paxs	825.34	Joback Method
dvisc	0.0000021	Paxs	898.44	Joback Method
dvisc	0.0000012	Paxs	971.54	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4475041&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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